Linear algebra for data science

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Abstract

This textbook presents the essential concepts from linear algebra of direct utility to analysis of large data sets. The theoretical foundations of the emerging discipline of Data Science are still being defined at present, but linear algebra is certainly one the cornerstones. Traditional presentations of linear algebra reflect its historical roots with a focus on linear systems and determinants, typically of small size. Presentation of the topic often links solutions of linear systems to posible intersections of lines or planes. Such an approach is ill-suited for data science in which the primary interest is in efficient description of large data sets, and automated extraction of regularity from the available data. Neither is the essence of solving a linear system presented as the information-conserving coordinate transformation that it actually represents when the system matrix is of full rank.

The emphasis in linear algebra presentation suggested by data science is quite different. The focus naturally shifts to the essential problem of efficient description of large data sets using a small, typically incomplete set of feature vectors. Linear algebra becomes the study of the basic operation of linear combination and its potential as a descriptor of large data sets. Rather than concentrate on the basis transformation represented by linear system solution, the focus shifts to maximal information compression. Instead of Gaussian elimination, the crucial algorithm becomes the singular value decomposition. The typical operation required is not to solve a linear system, but to construct low-dimensional approximations of the available data through projection and least squares.

Furthermore, computational exercises based on small matrices obscure the vitality and utility of linear algebra in data science of describing objects as disparate and information-rich as images, medical scans or sound recordings. To more faithfully portray the way linear algebra actually gets used in data science, this textbook is packaged with a complete software environment that contains extensive data sets, code snippets to carry out typical analysis, and procedures to transform heterogeneous data sources into standard linear algebra representations. Rather than relegate computational applications to isolated sections, the entire text is interspersed with practical examples using the Octave language, especially suited for linear algebra, and largely compatible with Matlab.

This textbook is drafted and meant to be worked through in TeXmacs, a scientific editing platform that features "live documents" with embedded computational examples constructed in freely available mathematical software systems such as Asymptote, Eukleides, Gnuplot, Maxima, and Octave. The most convenient method to ensure that these various systems work together as intended is to utilize this textbook within the Math@UNC virtual machine. A virtual machine is a program that runs on a physical computer and emulates another computer. Math@UNC is an Arch Linux environment built under VirtualBox, a freely available emulator that runs on Windows, OS X, Linux, and Solaris host computers. The main advantage of the Math@UNC system is pre-configuration of all Arch Linux and mathematical software settings, thus allowing students to learn usage of scientific software and mathematical concepts in a standard environment.

This textbook was developed for an intensive Maymester course that meets in twelve sessions of three hours each. The content organization reflects a desire to present crucial mathematical ideas and practical skills to students from various backgrounds who might be interested in data science. The key concepts required for mathematics students are present: matrix vector spaces, matrix factorizations, linear systems, eigenvalues. For a more general audience, these mathematical topics are also recast as addressing specific aspects of data: expressiveness, redundancy, efficiency, compression, partitioning. More than a simple relabeling, this reinterpretation allows for application of linear algebra operations to data far removed from the physial sciences or engineering. The text and its associated software environment considers data sets from visual art, music, biology, medicine, social sciences.

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CHAPTER 1

LINEAR COMBINATIONS

VECTORS AND MATRICES

1. Quantities

1.1. Numbers

Most scientific disciplines introduce an idea of the amount of some entity or property of interest. Furthermore, the amount is usually combined with the concept of a *number*, an abstraction of the observation that the two sets $A = \{\text{Mary, Jane, Tom}\}$ and $B = \{\text{apple, plum, cherry}\}$ seem quite different, but we can match one distinct person to one distinct fruit as in $\{\text{Mary}\longrightarrow\text{plum, Jane}\longrightarrow\text{apple, Tom}\longrightarrow\text{cherry}\}$. In contrast we cannot do the same matching of distinct persons to a distinct color from the set $\{\text{red, green}\}$, and one of the colors must be shared between two persons. Formal definition of the concept of a number from the above observations is surprisingly difficult since it would be self-referential due to the apperance of the numbers "one" and "two". Leaving this aside, the key concept is that of *quantity* of some property of interest that is expressed through a number. Several types of numbers have been introduced in mathematics to express different types of quantities, and the following will be used throughout this text:

- $\mathbb{N}$. The set of natural numbers, $\mathbb{N} = \{0, 1, 2, 3, \dots\}$, infinite and countable, $\mathbb{N}_+ = \{1, 2, 3, \dots\}$;
- $\mathbb{Z}$. The set of integers, $\mathbb{Z} = \{0, \pm 1, \pm 2, \pm 3, \dots\}$, infinite and countable;
- $\mathbf{Q}$. The set of rational numbers $\mathbb{Q} = \{p/q, p \in \mathbb{Z}, q \in \mathbb{N}_+\}$, infinite and countable;
- $\mathbb{R}$. The set of real numbers, infinite, not countable, can be ordered;
- $\mathbb{C}$. The set of complex numbers, $\mathbb{C} = \{x + iy, x, y \in \mathbb{R}\}$, infinite, not countable, cannot be ordered.

A computer has a finite amount of memory, hence cannot represent all numbers, but rather subsets of the above sets. Furthermore, computers internally use binary numbers composed of binary digits, or bits. Many computer number types are defined for specific purposes, and are often encountered in applications such as image representation or digital data acquisition. Here are the main types.

Subsets of $\mathbb{N}$. The number types `uint8`, `uint16`, `uint32`, `uint64` represent subsets of the natural numbers (unsigned integers) using 8, 16, 32, 64 bits respectively. An unsigned integer with b bits can store a natural number in the range from 0 to $2^b - 1$. Two arbitrary natural numbers, written as $\forall i, j \in \mathbb{N}$ can be added and will give another natural number, $k = i + j \in \mathbb{N}$. In contrast, addition of computer unsigned integers is only defined within the specific range 0 to $2^b - 1$.

```
octave] i=uint8(15); j=uint8(10); k=i+j
```

```
k = 25
```

```
octave] i=uint8(150); j=uint8(200); k=i+j
```

```
k = 255
```

```
octave] k=i-j
```

```
k = 0
```

```
octave]
```

Subsets of $\mathbb{Z}$. The number types `int8`, `int16`, `int32`, `int64` represent subsets of the integers. One bit is used to store the sign of the number, so the subset of $\mathbb{Z}$ that can be represented is from $1-2^{b-1}$ to $2^{b-1}-1$

```
octave] i=int8(100); j=int8(101); k=i+j
```

```
k = 127
```

```
octave] k=i-j
```

```
k = -1
```

```
octave]
```

Subsets of $\mathbb{Q}, \mathbb{R}, \mathbb{C}$. Computers approximate the real numbers through the set $\mathbb{F}$ of *floating point numbers*. Floating point numbers that use $b = 32$ bits are known as *single precision*, while those that use $b = 64$ are *double precision*. A floating point number $x \in \mathbb{F}$ is stored internally as $x = \pm.B_1B_2\ldots B_m \times 2^{\pm b_1 b_2 \ldots b_e}$ where B_i, $i = 1,\ldots,m$ are bits within the *mantissa* of length m, and b_j, $j = 1,\ldots,e$ are bits within the *exponent*, along with signs $\pm$ for each. The default number type is usually double precision, more concisely referred to `double`. Common constants such as e, π are predefined as `double`, can be truncated to `single`, and the number of displayed decimal digits is controlled by `format`. The function `disp(x)` displays its argument `x`.

```
octave] format long; disp([e pi])
```

```
   2.718281828459045   3.141592653589793
```

```
octave] disp([single(e) single(pi)])
```

```
   2.7182817   3.1415927
```

```
octave]
```

The approximation of the reals $\mathbb{R}$ by the floats $\mathbb{F}$ is characterized by: `realmax`, the largest float, `realmin` the smallest positive float, and `eps` known as *machine epsilon*. Machine epsilon highlights the differences between floating point and real numbers since it is defined as the largest number $\epsilon \in \mathbb{F}$ that satisfies $1+\epsilon = 1$. If $\varepsilon \in \mathbb{R}$ of course $1+\varepsilon = 1$ implies $\varepsilon = 0$, but floating points exhibit "granularity", in the sense that over a unit interval there are small steps that are indistinguishable from zero due to the finite number of bits available for a float. Machine epsilon is small, and floating point errors can usually be kept under control. Keep in mind that perfect accuracy is a mathematical abstraction, not encountered in nature. In fields as sociology or psychology 3 digits of accuracy are excellent, in mechanical engineering this might increase to 6 digits, or in electronic engineering to 8 digits. The most precisely known physical constant is the Rydberg constant known to 12 digits. The granularity of double precision expressed by machine epsilon is sufficient to represent natural phenomena.

```
octave] format short; disp([realmin realmax eps 1+eps])
```

```
   2.2251e-308   1.7977e+308    2.2204e-16    1.0000e+00
```

```
octave]
```

Within the reals certain operations are undefined such as $1/0$. Special float constants are defined to handle such situations: `Inf` is a float meant to represent infinity, and `NaN` ("not a number") is meant to represent an undefinable result of an arithmetic operation.

```
octave] warning("off"); disp([Inf 1/0 2*realmax NaN Inf-Inf Inf/Inf])
```

```
   Inf   Inf   Inf   NaN   NaN   NaN
```

```
octave]
```

Complex numbers $z \in \mathbb{C}$ are specified by two reals, in Cartesian form as $z = x + iy$, $x, y \in \mathbb{R}$ or in polar form as $z = \rho e^{i\theta}$, $\rho, \theta \in \mathbb{R}$, $\rho \geqslant 0$. The computer type complex is similarly defined from two floats and the additional constant I is defined to represent $\sqrt{-1} = i = e^{i\pi/2}$. Functions are available to obtain the real and imaginary parts within the Cartesian form, or the absolute value and argument of the polar form.

```
octave] z1=complex(1,1); z2=complex(1,-1); disp([z1+z2 z1/z2])
   2 + 0i   0 + 1i
octave] disp([real(z1) real(z2) real(z1+z2) real(z1/z2)])
   1   1   2   0
octave] disp([imag(z1) imag(z2) imag(z1+z2) imag(z1/z2)])
   1  -1   0   1
octave] disp([abs(z1) abs(z2) abs(z1+z2) abs(z1/z2)])
   1.4142   1.4142   2.0000   1.0000
octave] disp([arg(z1) arg(z2) arg(z1+z2) arg(z1/z2)])
   0.78540  -0.78540   0.00000   1.57080
octave] I-sqrt(-1)
ans = 0
octave]
```

Care should be exercised about the cummulative effect of many floating point errors. For instance, in an "irrational" numerical investigation of Zeno's paradox, one might want to compare the distance S_N traversed by step sizes that are scaled by $1/\pi$ starting from one to T_N, traversed by step sizes scaled by π starting from π^{-N}

$$S_N = 1 + \frac{1}{\pi} + \frac{1}{\pi^2} + \cdots + \frac{1}{\pi^N}, \; T_N = \frac{1}{\pi^N} + \frac{1}{\pi^{N-1}} + \cdots + 1.$$

In the reals the above two expressions are equal, $S_N = T_N$, but this is not verfied for all N when using floating point numbers. Lists of the values π^j, for the two orderings $j = 0, \ldots, N$, and $j = N, \ldots, 0$, can be generated and summed.

```
octave] N=10; S=pi.^(0:-1:-N); T=pi.^(-N:1:0); sum(S)==sum(T)
ans = 1
octave] N=15; S=pi.^(0:-1:-N); T=pi.^(-N:1:0); sum(S)==sum(T)
ans = 0
octave]
```

In the above numerical experiment a==b expresses an equality relationship which might evaluate as true denoted by 1, or false denoted by 0.

```
octave] disp([1==1 1==2])
  1  0
octave]
```

The above was called an "irrational" investigation since in Zeno's original paradox the scaling factor was 2 rather than π, and due to the binary representation used by floats equality always holds.

```
octave] N=30; S=2.^(0:-1:-N); T=2.^(-N:1:0); sum(S)==sum(T)
ans = 1
```

```
octave]
```

1.2. Quantities described by a single number

The above numbers and their computer approximations are sufficient to describe many quantities encountered in applications. Typical examples include:

- the position $x \in \mathbb{R}$ of a point on the unit line segment $[0, 1]$, approximated by the floating point number $\tilde{x} \in \mathbb{F}$, to within machine epsilon precision, $|x - \tilde{x}| \leqslant \epsilon$;
- the measure of resistance to change of the rate of motion known as *mass*, $m \in \mathbb{R}$, $m > 0$;
- the population of a large community expressed as a float $p \in \mathbb{F}$, even though for a community of individuals the population is a natural number, as in "the population of the United States is p = 328.2E6, i.e., 328.2 million".

In most disciplines, there is a particular interest in comparison of two quantities, and to facilitate such comparison a common reference is used known as a *standard unit*. For measurement of a length L, the meter $\ell = 1\,\mathrm{m}$ is a standard unit, as in the statement $L = 10\,\mathrm{m}$, that states that L is obtained by taking the standard unit ten times, $L = 10\ell$. The rules for carrying out such comparisons are part of the definition of real and rational numbers. These rules are formalized in the mathematical definition of a *field* $(F, +, \times)$ presented in the next chapter. Quantities that obey such rules, i.e., belong to a field, can be used in changes of scale and are called *scalars*. Not all numbers are scalars in this sense. For instance, the integers would not allow a scaling of 1:2 (halving the scale) even though 1,2 are integers.

1.3. Quantities described by multiple numbers

Other quantities require more than a single number. The distribution of population in the year 2000 among the alphabetically-ordered South American countries (Argentina, Bolivia,..,Venezuela) requires 12 numbers. These are placed together in a list known in mathematics as a *tuple*, in this case a 12-tuple $P = (p_1, p_2, \ldots, p_{12})$, with p_1 the population of Argentina, p_2 that of Bolivia, and so on. An analogous 12-tuple can be formed from the South American populations in the year 2020, say $Q = (q_1, q_2, ..., q_{12})$. Note that it is difficult to ascribe meaning to apparently plausible expressions such as $P + Q$ since, for instance, some people in the 2000 population are also in the 2020 population, and would be counted twice.

2. Vectors

2.1. Vector spaces

In contrast to the population 12-tuple example above, combining multiple numbers is well defined in operations such as specifying a position within a three-dimensional Cartesian grid, or determining the resultant of two forces in space. Both of these lead to the consideration of 3-tuples or *triples* such as the force (f_1, f_2, f_3). When combined with another force (g_1, g_2, g_3) the resultant is $(f_1 + g_1, f_2 + g_2, f_3 + g_3)$. If the force (f_1, f_2, f_3) is amplified by the scalar α and the force (g_1, g_2, g_3) is similarly scaled by β, the resultant becomes

$$\alpha(f_1, f_2, f_3) + \beta(g_1, g_2, g_3) = (\alpha f_1, \alpha f_2, \alpha f_3) + (\beta g_1, \beta g_2, \beta g_3) = (\alpha f_1 + \beta g_1, \alpha f_2 + \beta g_2, \alpha f_3 + \beta g_3).$$

It is useful to distinguish tuples for which scaling and addition is well defined from simple lists of numbers. In fact, since the essential difference is the behavior with respect to scaling and addition, the focus should be on these operations rather than the elements of the tuple.

The above observations underlie the definition of a *vector space* $\mathcal{V}$ by a set V whose elements satisfy certain scaling and addition properties, denoted all together by the 4-tuple $\mathcal{V} = (V, S, +, \cdot)$. The first element of the 4-tuple is a set whose elements are called *vectors*. The second element is a set of scalars, and the third is the vector addition operation. The last is the scaling operation, seen as multiplication of a vector by a scalar. The vector addition and scaling operations must satisfy rules suggested by positions or forces in three-dimensional space, which are listed in Table 1.1. In particular, a vector space requires definition of two distinguished elements: the zero vector $\mathbf{0} \in V$, and the identity scalar element $1 \in S$.

Addition rules for	$\forall \boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c} \in V$
$\boldsymbol{a} + \boldsymbol{b} \in V$	Closure
$\boldsymbol{a} + (\boldsymbol{b} + \boldsymbol{c}) = (\boldsymbol{a} + \boldsymbol{b}) + \boldsymbol{c}$	Associativity
$\boldsymbol{a} + \boldsymbol{b} = \boldsymbol{b} + \boldsymbol{a}$	Commutativity
$\boldsymbol{0} + \boldsymbol{a} = \boldsymbol{a}$	Zero vector
$\boldsymbol{a} + (-\boldsymbol{a}) = \boldsymbol{0}$	Additive inverse
Scaling rules for	$\forall \boldsymbol{a}, \boldsymbol{b} \in V, \forall x, y \in S$
$x\boldsymbol{a} \in V$	Closure
$x(\boldsymbol{a} + \boldsymbol{b}) = x\boldsymbol{a} + x\boldsymbol{b}$	Distributivity
$(x + y)\boldsymbol{a} = x\boldsymbol{a} + y\boldsymbol{a}$	Distributivity
$x(y\boldsymbol{a}) = (xy)\boldsymbol{a}$	Composition
$1\boldsymbol{a} = \boldsymbol{a}$	Scalar identity

Table 1.1. Vector space $\mathcal{V} = (V, S, +, \cdot)$ properties for arbitrary $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c} \in V$

The definition of a vector space reflects everyday experience with vectors in Euclidean geometry, and it is common to refer to such vectors by descriptions in a Cartesian coordinate system. For example, a position vector $\boldsymbol{r}$ within the plane can be referred through the pair of coordinates (x, y). This intuitive understanding can be made precise through the definition of a vector space $\mathscr{R}_2 = (\mathbb{R}^2, \mathbb{R}, +, \cdot)$, called the real 2-space. Vectors within $\mathscr{R}_2$ are elements of $\mathbb{R}^2 = \mathbb{R} \times \mathbb{R} = \{(x, y) \mid x, y \in \mathbb{R}\}$, meaning that a vector is specified through two real numbers, $\boldsymbol{r} \leftrightarrow (x, y)$. Addition of two vectors, $\boldsymbol{q} \leftrightarrow (s, t)$, $\boldsymbol{r} \leftrightarrow (x, y)$ is defined by addition of coordinates $\boldsymbol{q} + \boldsymbol{r} = (s + x, t + v)$. Scaling $\boldsymbol{r} \leftrightarrow (x, y)$ by scalar a is defined by $a\boldsymbol{r} \leftrightarrow (ax, ay)$. Similarly, consideration of position vectors in three-dimensional space leads to the definition of the $\mathscr{R}_3 = (\mathbb{R}^3, \mathbb{R}, +, \cdot)$, or more generally a real m-space $\mathscr{R}_m = (\mathbb{R}^m, \mathbb{R}, +, \cdot)$, $m \in \mathbb{N}$, $m > 0$.

Note however that there is no mention of coordinates in the definition of a vector space as can be seen from the list of properties in Table 1.1. The intent of such a definition is to highlight that besides position vectors, many other mathematical objects follow the same rules. As an example, consider the set of all continuous functions $C(\mathbb{R}) = \{f \mid f : \mathbb{R} \longrightarrow \mathbb{R}\}$, with function addition defined by the sum at each argument t, $(f + g)(t) = f(t) + g(t)$, and scaling by $a \in \mathbb{R}$ defined as $(af)(t) = af(t)$. Read this as: "given two continuous functions f and g, the function $f + g$ is defined by stating that its value for argument x is the sum of the two real numbers $f(t)$ and $g(t)$". Similarly: "given a continuous function f, the function af is defined by stating that its value for argument t is the product of the real numbers a and $f(t)$". Under such definitions $\mathcal{C}^0 = (C(\mathbb{R}), \mathbb{R}, +, \cdot)$ is a vector space, but quite different from $\mathscr{R}_m$. Nonetheless, the fact that both $\mathcal{C}^0$ and $\mathscr{R}_m$ are vector spaces can be used to obtain insight into the behavior of continuous functions from Euclidean vectors, and vice versa.

2.2. Real vector space $\mathscr{R}_m$

Column vectors. Since the real spaces $\mathscr{R}_m = (\mathbb{R}^m, \mathbb{R}, +, \cdot)$ play such an important role in themselves and as a guide to other vector spaces, familiarity with vector operations in $\mathscr{R}_m$ is necessary to fully appreciate the utility of linear algebra to a wide range of applications. Following the usage in geometry and physics, the m real numbers that specify a vector $\boldsymbol{u} \in \mathbb{R}^m$ are called the *components* of $\boldsymbol{u}$. The one-to-one correspondence between a vector and its components $\boldsymbol{u} \leftrightarrow (u_1, \ldots, u_m)$, is by convention taken to define an equality relationship,

$$\boldsymbol{u} = \begin{bmatrix} u_1 \\ \vdots \\ u_m \end{bmatrix}, \tag{1.1}$$

with the components arranged vertically and enclosed in square brackets. Given two vectors $\boldsymbol{u}, \boldsymbol{v} \in \mathbb{R}^m$, and a scalar $a \in \mathbb{R}$, vector addition and scaling are defined in $\mathscr{R}_m$ by real number addition and multiplication of components

$$\boldsymbol{u} + \boldsymbol{v} = \begin{bmatrix} u_1 \\ \vdots \\ u_m \end{bmatrix} + \begin{bmatrix} v_1 \\ \vdots \\ v_m \end{bmatrix} = \begin{bmatrix} u_1 + v_1 \\ \vdots \\ u_m + v_m \end{bmatrix}, a\boldsymbol{u} = a \begin{bmatrix} u_1 \\ \vdots \\ u_m \end{bmatrix} = \begin{bmatrix} au_1 \\ \vdots \\ au_m \end{bmatrix}. \tag{1.2}$$

The vector space $\mathscr{R}_m$ is defined using the real numbers as the set of scalars, and constructing vectors by grouping together m scalars, but this approach can be extended to any set of scalars S, leading to the definition of the vector

spaces $\mathcal{S}_n = (S^n, S, +, \cdot)$. These will often be referred to as *n-vector space of scalars*, signifying that the set of vectors is $V = S^n$.

To aid in visual recognition of vectors, the following notation conventions are introduced:

- vectors are denoted by lower-case bold Latin letters: $\boldsymbol{u}, \boldsymbol{v}$;
- scalars are denoted by normal face Latin or Greek letters: a, b, α, β;
- the components of a vector are denoted by the corresponding normal face with subscripts as in equation (1.1);
- related sets of vectors are denoted by indexed bold Latin letters: $\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots, \boldsymbol{u}_n$.

In Octave, successive components placed vertically are separated by a semicolon.

```
octave] [1; 2; -1; 2]
ans =

   1
   2
  -1
   2

octave]
```

The equal sign in mathematics signifies a particular equivalence relationship. In computer systems such as Octave the equal sign has the different meaning of *assignment*, that is defining the label on the left side of the equal sign to be the expression on the right side. Subsequent invocation of the label returns the assigned object. Components of a vector are obtained by enclosing the index in parantheses.

```
octave] u=[1; 2; -1; 2]; u
u =

   1
   2
  -1
   2

octave] u(3)
ans = -1
octave]
```

Row vectors. Instead of the vertical placement or components into one *column*, the components of could have been placed horizontally in one *row* $[\ u_1\ \ldots\ u_m\ ]$, that contains the same data, differently organized. By convention vertical placement of vector components is the preferred organization, and $\boldsymbol{u}$ shall denote a *column vector* henceforth. A transpose operation denoted by a T superscript is introduced to relate the two representations

$$\boldsymbol{u}^T = [\ u_1\ \ldots\ u_m\ ],$$

and $\boldsymbol{u}^T$ is the notation used to denote a *row vector*. In Octave, horizontal placement of successive components in a row is denoted by a space.

```
octave] uT=transpose(u)
uT =

   1   2  -1   2
```

```
octave] [1 2 -1 2]
ans =

   1   2  -1   2

octave] uT(4)
ans =  2
octave]
```

Compatible vectors. Addition of real vectors $\boldsymbol{u}, \boldsymbol{v} \in \mathbb{R}^m$ defines another vector $\boldsymbol{w} = \boldsymbol{u} + \boldsymbol{v} \in \mathbb{R}^m$. The components of $\boldsymbol{w}$ are the sums of the corresponding components of $\boldsymbol{u}$ and $\boldsymbol{v}$, $w_i = u_i + v_i$, for $i = 1, 2, \ldots, m$. Addition of vectors with different number of components is not defined, and attempting to add such vectors produces an error. Such vectors with different number of components are called *incompatible*, while vectors with the same number of components are said to be *compatible*. Scaling of $\boldsymbol{u}$ by a defines a vector $\boldsymbol{z} = a\boldsymbol{u}$, whose components are $z_i = a u_i$, for $i = 1, 2, \ldots, m$. Vector addition and scaling in Octave are defined using the + and * operators.

```
octave] uT=[1 0 1 2]; vT=[2 1 3 -1]; wT=uT+vT; disp(wT)
   3   1   4   1
octave] rT=[1 2]; uT+rT
operator +: nonconformant arguments (op1 is 1x4, op2 is 1x2)
octave] a=3; zT=a*uT; disp(zT)
   3   6  -3   6
octave]
```

2.3. Working with vectors

Ranges. The vectors used in applications usually have a large number of components, $m \gg 1$, and it is important to become proficient in their manipulation. Previous examples defined vectors by explicit listing of their m components. This is impractical for large m, and support is provided for automated generation for often-encountered situations. First, observe that Table 1.1 mentions one distinguished vector, the zero element that is a member of any vector space $\mathbf{0} \in V$. The zero vector of a real vector space $\mathscr{R}_m$ is a column vector with m components, all of which are zero, and a mathematical convention for specifying this vector is $\mathbf{0}^T = [\ 0\ \ 0\ \ \ldots\ \ 0\ ] \in \mathbb{R}^m$. This notation specifies that transpose of the zero vector is the row vector with m zero components, also written through explicit indexing of each component as $\mathbf{0}_i = 0$, for $i = 1, \ldots, m$. Keep in mind that the zero vector $\mathbf{0}$ and the zero scalar 0 are different mathematical objects. The ellipsis symbol in the mathematical notation is transcribed in Octave by the notion of a range, with `1:m` denoting all the integers starting from 1 to m, organized as a row vector. The notation is extended to allow for strides different from one, and the mathematical ellipsis $i = m, m-1,...,1$ is denoted as `m:-1:1`. In general `r:s:t` denotes the set of numbers $\{r, r+s, \ldots, r+ns\}$ with $r + ns \leqslant t$, and r, s, t real numbers and n a natural number, $r, s, t \in \mathbb{R}$, $n \in \mathbb{N}$. If there is no natural number n such that $r + ns \leqslant t$, an empty vector with no components is returned.

```
octave] m=4; disp(1:m)
   1   2   3   4
octave] disp(m:-1:2)
   4   3   2
octave] r=0; s=0.2; t=1; disp(r:s:t)
    0.00000    0.20000    0.40000    0.60000    0.80000    1.00000
```

```
octave] r=0; s=0.3; t=1; disp(r:s:t)
    0.00000    0.30000    0.60000    0.90000
octave] r=0; s= -0.2; t=1; disp(r:s:t)
[](1x0)
octave]
```

An efficient, expressive feature of many software systems including Octave is to use ranges as indices to a vector, as shown below for the definition of $\mathbf{0}\in\mathbb{R}^4$. Note that the index range `i` is organized as a row, and a transpose operation must be applied to obtain `z` as a column vector.

```
octave] m=4; i=1:m; z(i)=i.^i; z=transpose(z); disp(z)
     1
     4
    27
   256
octave] i
i =

   1   2   3   4

octave] disp(transpose(z))
   0   0   0   0
octave]
```

Visualization. A component-by-component display of a vector becomes increasingly unwieldy as the number of components m becomes large. For example, the numbers below seem an inefficient way to describe the sine function.

```
octave]  t=0:0.1:1.5; disp(sin(t))
  Columns 1 through 8:

   0.00000   0.09983   0.19867   0.29552   0.38942   0.47943   0.56464   0.64422

  Columns 9 through 16:

   0.71736   0.78333   0.84147   0.89121   0.93204   0.96356   0.98545   0.99749
octave]
```

Indeed, such a piece-by-piece approach is not the way humans organize large amounts of information, preferring to conceptualize the data as some other entity: an image, a sound excerpt, a smell, a taste, a touch, a sense of balance, or relative position. All seven of these human senses will be shown to allow representation by linear algebra concepts, including representation by vectors.

As a first example consider *visualization*, the process of transforming data into a sight perception. A familiar example is constructing a plot of the graph of a function. Recall that in mathematics the *graph of a function* $f: X\longrightarrow Y$ relating elements of the *domain* X to those in *codomain* Y is a set of ordered pairs $G_f=\{(x,y)\mid y=f(x), x\in X\}$. For a commonly encountered function such as $\sin: [0,2\pi)\longrightarrow[-1,1]$, the graph $G_{\sin}=\{(x,\sin(x))\mid x\in[0,2\pi)\}$ contains an uncountably infinite number of elements, and obviously cannot be explicitly listed. The sine function is continuous, meaning that no matter how small an open interval (c,d) within the function codomain $[-1,1]$ one considers, there exists an interval (a,b) in the function domain $[0,2\pi]$ whose image by the sine function

is contained in (c,d). In mathematical "$\delta-\varepsilon$" notation this is stated as: $\forall\varepsilon>0, \exists\delta_\varepsilon, \mid x_1-x_0\mid<\delta_\varepsilon \Longrightarrow \mid \sin(x_1)-\sin(x_0)\mid <\varepsilon$. This mathematical notation is concise and precise, but perceptive mainly to the professional mathematician. A more intuitive visualization of continuity is obtained by approximating the graph of a function $f: X \longrightarrow Y$ by a finite set of samples, $G_f^m = \{(x_i, y_i) \mid x_i \in X, y_i = f(x_i), i = 1, \ldots, m, m \in \mathbb{N}\}$. Strictly speaking, the sampled graph G_f^m would indicate jumps interpretable as discontinuities, but when plotting the points human sight perception conveys a sense of continuity for large sample sizes, $m \gg 1$. For the sine function example, consider sampling the domain $[0, 2\pi)$ with a step size $h = 2\pi/m$, $m \gg 1$. To obtain a visual representation of the sampled sine function the Octave `plot` function can be used to produce a figure that will appear in another window, interactively investigated, and subsequently closed. For large m one cannot visually distinguish the points in the graph sample, though this is apparent for smaller sample sizes. This is shown below by displaying a subrange of the sampled points with stride s. This example also shows the procedure to save a permanent copy of the displayed figure through the Octave `print -deps` command that places the currently displayed plot into an Encapsulated Postscript file. The generated figure file can be linked to a document as shown here in Figure 1.1, in which both plots render samples of the graph of the sine function, but the one with large m is perceived as being continuous.

```
octave] m=1000; h=2*pi/m; x=(0:m-1)*h;
octave] y=sin(x); plot(x,y);
octave] close;
octave] s=50; i=1:s:m; xs=x(i); ys=y(i);
octave] plot(x,y,'b',xs,ys,'bo');
octave] print -depsc L01Fig01.eps;
octave] close;
octave]
```

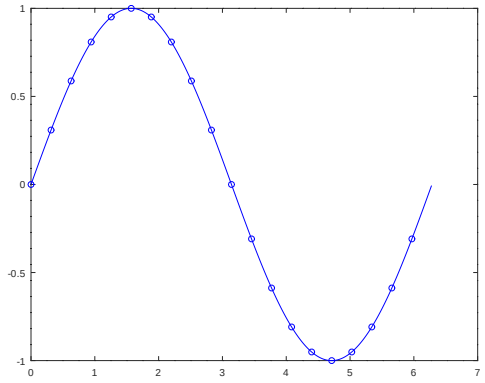


Figure 1.1. Visualization of vectors of sampled function graphs.

3. Matrices

3.1. Forming matrices

The real numbers themselves form the vector space $\mathscr{R}_1 = (\mathbb{R}, \mathbb{R}, +, \cdot)$, as does any field of scalars, $\mathscr{S}_1 = (S, S, +, \cdot)$. Juxtaposition of m real numbers has been seen to define the new vector space $\mathscr{R}_m$. This process of juxtaposition can be continued to form additional mathematical objects. A *matrix* is defined as a juxtaposition of compatible vectors. As an example, consider n vectors $\boldsymbol{a}_1, \boldsymbol{a}_2, \ldots, \boldsymbol{a}_n \in V$ within some vector space $\mathscr{V} = (V, S, +, \cdot)$. Form a matrix by placing the vectors into a row,

$$\boldsymbol{A} = \left[\begin{array}{cccc} \boldsymbol{a}_1 & \boldsymbol{a}_2 & \ldots & \boldsymbol{a}_n \end{array}\right]. \tag{1.3}$$

To aid in visual recognition of a matrix, upper-case bold Latin letters will be used to denote matrices. The columns of a matrix will be denoted by the corresponding lower-case bold letter with a subscripted index as in equation (1.3). Note that the number of columns in a matrix can be different from the number of components in each column, as would be the case for matrix $\boldsymbol{A}$ from equation (1.3) when choosing vectors from, say, the real space $\mathscr{R}_m$, $\boldsymbol{a}_1, \boldsymbol{a}_2, \ldots, \boldsymbol{a}_n \in \mathbb{R}^m$.

Vectors were seen to be useful juxtapositions of scalars that could describe quantities a single scalar could not: a position in space, a force in physics, or a sampled function graph. The crucial utility of matrices is their central role in providing a description of new vectors other then their column vectors, and is suggested by experience with Euclidean spaces.

3.2. Identity matrix

Consider first $\mathscr{R}_1$, the vector space of real numbers. A position vector $\boldsymbol{r} \in \mathscr{R}_1$ on the real axis is specified by a single scalar component, $\boldsymbol{r} = [x]$, $x \in \mathbb{R}$. Read this to mean that the position $\boldsymbol{r}$ is obtained by traveling x units from the origin at position vector $\boldsymbol{0} = [0]$. Look closely at what is meant by "unit" in this context. Since x is a scalar, the mathematical expression $\boldsymbol{r} = \boldsymbol{0} + x$ has no meaning, as addition of a vector to a scalar has not been defined. Recall that scalars were introduced to capture the concept of scaling of a vector, so in the context of vector spaces they always appear as multiplying some vector. The correct mathematical description is $\boldsymbol{r} = \boldsymbol{0} + x\,\boldsymbol{e}$, where $\boldsymbol{e}$ is the unit vector $\boldsymbol{e} = [1]$. Taking the components leads to $r_1 = 0_1 + x e_1$, where $r_1, 0_1, e_1$ are the first (and in this case only) components of the $\boldsymbol{r}, \boldsymbol{0}, \boldsymbol{e}$ vectors. Since $r_1 = x$, $0_1 = 0$, $e_1 = 1$, one obtains the identity $x = 0 + x \cdot 1$.

Now consider $\mathscr{R}_2$, the vector space of positions in the plane. Repeating the above train of thought leads to the identification of two direction vectors $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$

$$\boldsymbol{r} = \begin{bmatrix} x \\ y \end{bmatrix} = x \begin{bmatrix} 1 \\ 0 \end{bmatrix} + y \begin{bmatrix} 0 \\ 1 \end{bmatrix} = x\,\boldsymbol{e}_1 + y\,\boldsymbol{e}_2,\ \boldsymbol{e}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix},\ \boldsymbol{e}_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

```
octave] x=2; y=4; e1=[1; 0]; e2=[0; 1]; r=x*e1+y*e2
```

```
r =

   2
   4
```

```
octave]
```

Continuing the procees to $\mathscr{R}_m$ gives

$$\boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix} = x_1\,\boldsymbol{e}_1 + x_2\,\boldsymbol{e}_2 + \cdots + x_m\,\boldsymbol{e}_m,\ \boldsymbol{e}_1 = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix},\ \boldsymbol{e}_2 = \begin{bmatrix} 0 \\ 1 \\ \vdots \\ 0 \\ 0 \end{bmatrix},\ \ldots,\ \boldsymbol{e}_m = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}.$$

For arbitrary m, the components are now $x_1, x_2, \ldots, x_m$ rather than the alphabetically ordered letters common for $m = 2$ or $m = 3$. It is then consistent with the adopted notation convention to use $\boldsymbol{x} \in \mathscr{R}_m$ to denote the position vector whose components are $(x_1, \ldots, x_m)$. The basic idea is the same as in the previous cases: to obtain a position vector scale direction $\boldsymbol{e}_1$ by x_1, $\boldsymbol{e}_2$ by x_2,..., $\boldsymbol{e}_m$ by x_m, and add the resulting vectors.

Juxtaposition of the vectors $\boldsymbol{e}_1, \boldsymbol{e}_2, \ldots, \boldsymbol{e}_m$ leads to the formation of a matrix of special utility known as the *identity matrix*

$$\boldsymbol{I} = [\ \boldsymbol{e}_1\ \ \boldsymbol{e}_2\ \ \ldots\ \ \boldsymbol{e}_m\ ].$$

The identity matrix is an example of a matrix in which the number of column vectors n is equal to the number of components in each column vector $m = n$. Such matrices with equal number of columns and rows are said to be *square*. Due to entrenched practice an exception to the notation convention is made and the identity matrix is denoted by $\boldsymbol{I}$, but its columns are denoted the indexed bold-face of a different lower-case letter, $\boldsymbol{e}_1, \ldots, \boldsymbol{e}_m$. If it becomes necessary to explicitly state the number of columns in $\boldsymbol{I}$, the notation $\boldsymbol{I}_m$ is used to denote the identity matrix with m columns, each with m components.

4. Linear combinations

4.1. Linear combination as a matrix-vector product

The expression $\boldsymbol{x} = x_1\,\boldsymbol{e}_1 + x_2\,\boldsymbol{e}_2 + \cdots + x_m\,\boldsymbol{e}_m$ expresses the idea of scaling vectors within a set and subsequent addition to form a new vector $\boldsymbol{x}$. The matrix $\boldsymbol{I} = [\ \boldsymbol{e}_1\ \ \boldsymbol{e}_2\ \ \ldots\ \ \boldsymbol{e}_m\ ]$ groups these vectors together in a single entity, and the

scaling factors are the components of the vector $\boldsymbol{x}$. To bring all these concepts together it is natural to consider the notation

$$\boldsymbol{x} = \boldsymbol{I}\boldsymbol{x},$$

as a generalization of the scalar expression $x = 1 \cdot x$. It is clear what the operation $\boldsymbol{I}\boldsymbol{x}$ should signify: it should capture the vector scaling and subsequent vector addition $x_1\,\boldsymbol{e}_1 + x_2\,\boldsymbol{e}_2 + \cdots + x_m\,\boldsymbol{e}_m$. A specific meaning is now ascribed to $\boldsymbol{I}\boldsymbol{x}$ by identifying two definitions to one another.

Linear combination. Repeateadly stating "vector scaling and subsequent vector addition" is unwieldy, so a special term is introduced for some given set of vectors $\{\boldsymbol{a}_1, \ldots, \boldsymbol{a}_n\}$.

DEFINITION. (LINEAR COMBINATION) . *The linear combination of vectors $\boldsymbol{a}_1, \boldsymbol{a}_2, \ldots, \boldsymbol{a}_n \in V$ with scalars $x_1, x_2, \ldots, x_n \in S$ in vector space $(V, S, +, \cdot)$ is the vector $\boldsymbol{b} = x_1\,\boldsymbol{a}_1 + x_2\,\boldsymbol{a}_2 + \ldots x_n\,\boldsymbol{a}_n$.*

Matrix-vector product. Similar to the grouping of unit vectors $\boldsymbol{e}_1, \ldots, \boldsymbol{e}_m$ into the identity matrix $\boldsymbol{I}$, a more concise way of referring to arbitrary vectors $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_n$ from the same vector space is the matrix $\boldsymbol{A} = [\ \boldsymbol{a}_1\ \ \boldsymbol{a}_2\ \ \ldots\ \ \boldsymbol{a}_n\ ]$. Combining these observations leads to the definition of a matrix-vector product.

DEFINITION. (MATRIX-VECTOR PRODUCT) . *In the vector space $(V, S, +, \cdot)$, the product of matrix $\boldsymbol{A} = [\ \boldsymbol{a}_1\ \ \boldsymbol{a}_2\ \ \ldots\ \ \boldsymbol{a}_n\ ]$ composed of columns $\boldsymbol{a}_1, \boldsymbol{a}_2, \ldots, \boldsymbol{a}_n \in V$ with the vector $\boldsymbol{x} \in S_n$ whose components are scalars $x_1, x_2, \ldots, x_n \in S$ is the linear combination $\boldsymbol{b} = x_1\,\boldsymbol{a}_1 + x_2\,\boldsymbol{a}_2 + \ldots x_n\,\boldsymbol{a}_n = \boldsymbol{A}\boldsymbol{x} \in V$.*

4.2. Linear algebra problem examples

Linear combinations in E_2. Consider a simple example that leads to a common linear algebra problem: decomposition of forces in the plane along two directions. Suppose a force is given in terms of components along the Cartesian x, y-axes, $\boldsymbol{b} = b_x\,\boldsymbol{e}_x + b_y\,\boldsymbol{e}_y$, as expressed by the matrix-vector multiplication $\boldsymbol{b} = \boldsymbol{I}\boldsymbol{b}$. Note that the same force could be obtained by linear combination of other vectors, for instance the normal and tangential components of the force applied on an inclined plane with angle θ, $\boldsymbol{b} = x_t\,\boldsymbol{e}_t + x_n\,\boldsymbol{e}_n$, as in Figure 1.2. This defines an alternate reference system for the problem. The unit vectors along these directions are

$$\boldsymbol{t} = \begin{bmatrix} \cos\theta \\ \sin\theta \end{bmatrix}, \boldsymbol{n} = \begin{bmatrix} -\sin\theta \\ \cos\theta \end{bmatrix},$$

and can be combined into a matrix $\boldsymbol{A} = [\ \boldsymbol{t}\ \ \boldsymbol{n}\ ]$. The value of the components (x_t, x_n) are the scaling factors and can be combined into a vector $\boldsymbol{x} = [\ x_t\ \ x_n\ ]^T$. The same force must result irrespective of whether its components are given along the Cartesian axes or the inclined plane directions leading to the equality

$$\boldsymbol{I}\boldsymbol{b} = \boldsymbol{b} = \boldsymbol{A}\boldsymbol{x}. \tag{1.4}$$

Interpret equation (1.4) to state that the vector $\boldsymbol{b}$ could be obtained either as a linear combination of $\boldsymbol{I}$, $\boldsymbol{b} = \boldsymbol{I}\boldsymbol{b}$, or as a linear combination of the columns of $\boldsymbol{A}$, $\boldsymbol{b} = \boldsymbol{A}\boldsymbol{x}$. Of course the simpler description seems to be $\boldsymbol{I}\boldsymbol{b}$ for which the components are already known. But this is only due to an arbitrary choice made by a human observer to define the force in terms of horizontal and vertical components. The problem itself suggests that the tangential and normal components are more relevant; for instance a friction force would be evaluated as a scaling of the normal force. The components in this more natural reference system are not known, but can be determined by solving the vector equality $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$, known as a *linear system of equations*. Procedures to carry this out will be studied in more detail later, but Octave provides an instruction for this common problem, the backslash operator, as in `x=A\b`.

```
octave] ex=[1; 0]; ey=[0; 1];
octave] b=[0.2; 0.4]; I=[ex ey]; I*b
ans =

   0.20000
   0.40000

octave] th=pi/6; c=cos(th); s=sin(th);
octave] tvec=[c; s]; nvec=[-s; c];
octave] A=[tvec nvec];
octave] x=A\b
x =

   0.37321
   0.24641

octave] [x(1)*tvec x(2)*nvec]
ans =

   0.32321  -0.12321
   0.18660   0.21340

octave]
```

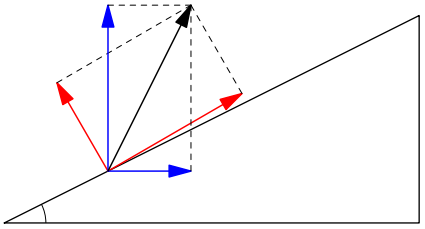


Figure 1.2. Alternative decompositions of force on inclined plane.

Linear combinations in $\mathcal{R}_m$ and $C^0[0,2\pi)$. Linear combinations in a real space can suggest properties or approximations of more complex objects such as continuous functions. Let $C^0[0,2\pi) = (C[0,2\pi), \mathbb{R}, +, \cdot)$ denote the vector space of continuous functions that are periodic on the interval $[0,2\pi)$, $C[0,\pi) = \{f \mid f\colon \mathbb{R} \longrightarrow \mathbb{R}, f(t) = f(t+2\pi)\}$. Recall that vector addition is defined by $(f+g)(t) = f(t) + g(t)$, and scaling by $(af)(t) = af(t)$, for $f, g \in C[0,2\pi)$, $a \in \mathbb{R}$. Familiar functions within this vector space are $\sin(kt)$, $\cos(kt)$ with $k \in \mathbb{N}$, and these can be recognized to intrinsically represent periodicity on $[0,2\pi)$, a role analogous to the normal and tangential directions in the inclined plane example.

Define now another periodic function $b(t+2\pi) = b(t)$ by repeating the values $b(t) = t(\pi - t)(2\pi - t)$ from the interval $[0,2\pi)$ on all intervals $[2p\pi, 2(p+1)\pi\,]$, for $p \in \mathbb{Z}$. The function b is not given in terms of the "naturally" periodic functions $\sin(kt)$, $\cos(kt)$, but could it thus be expressed? This can be stated as seeking a linear combination $b(t) = \sum_{k=1}^{\infty} x_k \sin(kt)$, as studied in Fourier analysis. The coefficients x_k could be determined from an analytical formula involving calculus operations $x_k = \frac{1}{\pi}\int_0^{2\pi} b(t)\sin(kt)\,\mathrm{d}t$, but we'll seek an approximation using a linear combination of n terms

$$b(t) \cong \sum_{k=1}^{n} x_k \sin(kt), A(t) = [\ \sin(t)\ \ \sin(2t)\ \ \ldots\ \ \sin(nt)\ ], A\colon \mathbb{R} \longrightarrow \mathbb{R}^n.$$

Organize this as a matrix vector product $b(\boldsymbol{t}) \cong A(\boldsymbol{t})\,\boldsymbol{x}$, with

$$A(\boldsymbol{t}) = [\ \sin(\boldsymbol{t})\ \ \sin(2\boldsymbol{t})\ \ \ldots\ \ \sin(n\boldsymbol{t})\ ], \boldsymbol{x} = [\ x_1\ \ x_2\ \ \ldots\ \ x_n\ ]^T \in \mathbb{R}^n.$$

The idea is to sample the column vectors of $A(\boldsymbol{t})$ at the components of the vector $\boldsymbol{t} = [\ t_1\ \ t_2\ \ \ldots\ \ t_m\ ]^T \in \mathbb{R}^m$, $t_j = (j-1)h$, $j = 1, 2, \ldots, m$, $h = \pi/m$. Let $\boldsymbol{b} = b(\boldsymbol{t})$, and $\boldsymbol{A} = A(\boldsymbol{t})$, denote the so-sampled b, A functions leading to the definition of a vector $\boldsymbol{b} \in \mathbb{R}^m$ and a matrix $\boldsymbol{A} \in \mathbb{R}^{m\times n}$. There are n coefficients available to scale the column vectors of $\boldsymbol{A}$, and $\boldsymbol{b}$ has m components. For $m > n$ it is generally not possible to find $\boldsymbol{x}$ such that $\boldsymbol{Ax}$ would exactly equal $\boldsymbol{b}$, but as seen later the condition to be as close as possible to $\boldsymbol{b}$ leads to a well defined solution procedure. This is known as a least squares problem and is automatically applied in the Octave `x=A\b` instruction when the matrix `A` is not square. As seen in the following numerical experiment and Figure 1.3, the approximation is excellent even though the information

conveyed by $m = 1000$ samples of $b(t)$ is now much more efficiently stored in the form chosen for the columns of $\boldsymbol{A}$ and the $n = 11$ scaling coefficients that are the components of $\boldsymbol{x}$.

```
octave] m=1000; h=2*pi/m; j=1:m;
octave] t(j)=(j-1)*h; t=transpose(t);
octave] n=5; A=[];
octave] for k=1:n
          A = [A sin(k*t)];
        end
octave] bt=t.*(pi-t).*(2*pi-t);
octave] x=A\bt;
octave] b=A*x;
octave] s=50; i=1:s:m;
        ts=t(i); bs=bt(i);
        plot(ts,bs,'ok',t,b,'r');
octave] print -depsc L01Fig02.eps
octave] close;
```

```
octave]
```

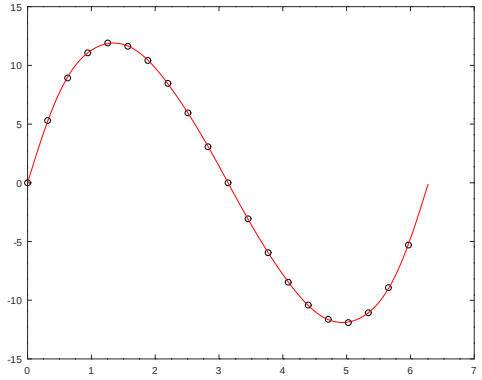


Figure 1.3. Comparison of least squares approximation (red line) with samples of exact function $b(t)$.

5. Vectors and matrice in data science

The above examples highlight some essential aspects of linear algebra in the context of data science applications.

- Vectors organize information that cannot be expressed as a single number and for which there exists a concept of scaling and addition.
- Matrices group together multiple vectors.
- The matrix-vector product expresses a linear combination of the column vectors of the matrix.
- Solving a linear system $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b} = \boldsymbol{I}\boldsymbol{b}$, to find $\boldsymbol{x} \in \mathbb{R}^m$ for given $\boldsymbol{b} \in \mathbb{R}^m$, re-expresses the linear combination

  $$\boldsymbol{b} = b_1\boldsymbol{e}_1 + \cdots + b_m\boldsymbol{e}_m, \boldsymbol{I} = \left[\begin{array}{cccc} \boldsymbol{e}_1 & \boldsymbol{e}_2 & \ldots & \boldsymbol{e}_m \end{array}\right],$$

  as another linear combination

  $$\boldsymbol{b} = x_1\boldsymbol{a}_1 + x_2\boldsymbol{a}_2 + \ldots x_n\boldsymbol{a}_n, \boldsymbol{A} = \left[\begin{array}{cccc} \boldsymbol{a}_1 & \boldsymbol{a}_2 & \ldots & \boldsymbol{a}_n \end{array}\right].$$

  For certain problems the linear combination $\boldsymbol{A}\boldsymbol{x}$ might be more insightful, but the above transformation is information-preserving, with $\boldsymbol{b}, \boldsymbol{x}$ both having the same number of components.
- Finding the best approximation of some given $\boldsymbol{b} \in \mathbb{R}^m$ by a linear combination $\boldsymbol{A}\boldsymbol{x}$ of the n column vectors of $\boldsymbol{A} \in \mathbb{R}^{m \times n}$ is known as a least squares problem and transforms the information from the m components of $\boldsymbol{b}$ into n components of $\boldsymbol{x}$, and knowledge of the form of the column vectors. If $m > n$ and the form of the columns of $\boldsymbol{A}$ can be succintly stated, the transformation compresses information.

Data science seeks to extract regularity directly from available data, not necessarily invoking any additional hypotheses. The typical scenario is that immense amounts of data are available, with limited capability of human analysis. In this context it is apparent that the least squares problem is of greater interest than solving a linear system with a square matrix. It should also be clear that while computation by hand of small examples is useful to solidify theroretical concepts, it is essential to become proficient in the use of software that can deal with large data sets, such as Octave.

LINEAR MAPPINGS

1. Functions

1.1. Relations

The previous chapter focused on mathematical expression of the concept of *quantification*, the act of associating human observation with measurements, as a first step of scientific inquiry. Consideration of different types of quantities led to various types of numbers, vectors as groupings of numbers, and matrices as groupings of vectors. Symbols were introduced for these quantities along with some intial rules for manipulating such objects, laying the foundation for an *algebra* of vectors and matrices. Science seeks to not only observe, but to also explain, which now leads to additional operations for working with vectors and matrices that will define the framework of *linear algebra*.

Explanations within scientific inquiry are formulated as hypotheses, from which predictions are derived and tested. A widely applied mathematical transcription of this process is to organize hypotheses and predictions as two sets X and Y, and then construct another set R of all of the instances in which an element of X is associated with an element in Y. The set of all possible instances of $x \in X$ and $y \in Y$, is the *Cartesian product* of X with Y, denoted as $X \times Y = \{(x,y) \mid x \in X, y \in Y\}$, a construct already encountered in the definition of the real 2-space $\mathscr{R}_2 = (\mathbb{R}^2, \mathbb{R}, +, \cdot)$ where $\mathbb{R}^2 = \mathbb{R} \times \mathbb{R}$. Typically, not all possible tuples $(x,y) \in X \times Y$ are relevant leading to the following definition.

DEFINITION. (RELATION) . *A relation R between two sets X, Y is a subset of the Cartesian product $X \times Y$, $R \subseteq X \times Y$.*

Similar to the difficulties encountered in attempting rigorous definition of a natural number, careful parsing of the above definition also would reveal self-references since the member of symbol $\in$, and the subset of symbol $\subseteq$ are both themselves examples of relations. As before, this is set aside to concetrate on the key concept of *associating an input $x \in X$ with an output $y \in Y$*. Associating an output to an input is also useful, leading to the definition of an *inverse relation* as $R^{-1} \subseteq Y \times X$, $R^{-1} = \{(y,x) \mid (x,y) \in R\}$. Note that an inverse exists for any relation, and the inverse of an inverse is the original relation, $(R^{-1})^{-1} = R$. From the above, a relation is a triplet (a tuple with three elements), (X, Y, R), that will often be referred to by just its last member R.

Computers can be programmed to work not only with numbers as Octave does, but also with general symbols as exemplified by another freely available software package called Maxima. Most data science applications involve numerical computation, but some knowledge of symbolic computation is also useful, as when working with sets that often arises in data classification. The colon symbol denotes assignment in Maxima, and sets can be defined using curly braces with automatic elimination of repeated elements. All common set manipulations are provided, such as the Cartesian product $\times$, and element of $\in$. operations.

```
%i1] X: {a,b,c,b,a}
```

(%o1) $\{a, b, c\}$

```
%i2] Y: {alpha,beta,gamma}
```

(%o2) $\{\alpha,\beta,\gamma\}$

```
%i3] XxY: cartesian_product(X,Y)
```

(%o3) $\{[a,\alpha],[a,\beta],[a,\gamma],[b,\alpha],[b,\beta],[b,\gamma],[c,\alpha],[c,\beta],[c,\gamma]\}$

```
%i4] [elementp([a,alpha],XxY), elementp([alpha,a],XxY)]
```

(%o4) [**true**, **false**]

```
%i5]
```

Associate the first three Latin and Greek letters by defining $R = \{(a,\alpha),(b,\beta),(c,\gamma)\}$. This is a relation between $X = \{a,b,c\}$ and $Y = \{\alpha,\beta,\gamma\}$ since it is a subset of $X \times Y$, which can be checked by defining a function that checks whether some $r \in R$ is also an element of $X \times Y$. Maxima functions are defined using the `:=` operator, and `map` applies a function to all elements of a set.

```
%i10] R: {[a,alpha],[b,beta],[c,gamma]}$
      verifyXxY(r):= elementp(r,XxY)$
      map(verifyXxY,R)
```

(%o12) {**true**}

```
%i13]
```

Suppose that the Greek alphabet ordering is not known, and a might conceivably be associated to any of α,β,γ. This defines another relation $S = \{(a,\alpha),(a,\beta),(a,\gamma)\}$. Finally consider possible reorderings of the Greek alphabet, formulated as relationships between Y and itself, with $P = \{(\alpha,\beta),(\beta,\gamma),(\gamma,\alpha)\}$ and $I = \{(\alpha,\alpha),(\beta,\beta),(\gamma,\gamma)\}$ two such possible reorderings. The relations R, S, P, I defined here will be used to exemplify various properties below.

```
%i13] S: {[a,alpha],[a,beta],[a,gamma]}$
      YxY: cartesian_product(Y,Y)$ verifyYxY(r):= elementp(r,YxY)$
      P: {[alpha,beta],  [beta,gamma], [gamma,alpha]}$
      I: {[alpha,alpha], [beta,beta],  [gamma,gamma]}$
      [map(verifyXxY,S), map(verifyYxY,P), map(verifyYxY,I)]
```

(%o18) [{**true**},{**true**},{**true**}]

Homogeneous relations. Many types of relations are defined in mathematics and encountered in linear algebra, and establishing properties of specific relations is an important task within data science. A commonly encountered type of relationship is from a set onto itself, known as a *homogeneous* relation. Among the above-defined relations $P, I \subseteq Y \times Y$ are homogeneous, while $R, S \subseteq X \times Y$ are not. For homogeneous relations $H \subseteq A \times A$, it is common to replace the set membership notation $(a,b) \in H$ to state that $a \in A$ is in relationship H with $b \in A$, with a binary operator notation $a \overset{H}{\sim} b$. Familiar examples include the equality and less than relationships between reals, $E, L \subseteq \mathbb{R} \times \mathbb{R}$, in which $(a,b) \in E$ is replaced by $a = b$, and $(a,b) \in L$ is replaced by $a < b$. The equality relationship is its own inverse, and the inverse of the less than relationship is the greater than relation $G \subseteq \mathbb{R} \times \mathbb{R}$, $G = L^{-1}$, $a < b \implies b > a$. Homogeneous relations $H \subseteq A \times A$ are classified according to the following criteria.

Reflection. Relation H is reflexive if $(a,a) \in H$ for any $a \in A$. The equality relation $E \subseteq \mathbb{R} \times \mathbb{R}$ is reflexive, $\forall a \in A$, $a = a$, the less than relation $L \subseteq \mathbb{R} \times \mathbb{R}$ is not, $1 \in R, 1 \nless 1$.

Symmetry. Relation H is symmetric if $(a,b) \in H$ implies that $(b,a) \in H$, $(a,b) \in H \implies (b,a) \in H$. The equality relation $E \subseteq \mathbb{R} \times \mathbb{R}$ is symmetric, $a = b \implies b = a$, the less than relation $L \subseteq \mathbb{R} \times \mathbb{R}$ is not, $a < b \nRightarrow b < a$.

Anti-symmetry. Relation H is anti-symmetric if $(a,b) \in H$ for $a \neq b$, then $(b,a) \notin H$. The less than relation $L \subseteq \mathbb{R} \times \mathbb{R}$ is antisymmetric, $a < b \implies b \neq a$.

Transitivity. Relation H is transitive if $(a,b) \in H$ and $(b,c) \in H$ implies $(a,c) \in H$. for any $a \in A$. The equality relation $E \subseteq \mathbb{R} \times \mathbb{R}$ is transitive, $a = b \wedge b = c \implies a = c$, as is the less than relation $L \subseteq \mathbb{R} \times \mathbb{R}$, $a < b \wedge b < c \implies a < c$.

Certain combinations of properties often arise. A homogeneous relation that is reflexive, symmetric, and transitive is said to be an *equivalence relation*. Equivalence relations include equality among the reals, or congruence among triangles. A homogeneous relation that is reflexive, anti-symmetric and transitive is a *partial order relation*, such as the less than or equal relation between reals. Finally, a homogeneous relation that is anti-symmetric and transitive is an *order relation*, such as the less than relation between reals.

1.2. Functions

Functions between sets X and Y are a specific type of relationship that often arise in science. For a given input $x \in X$, theories that predict a single possible output $y \in Y$ are of particular scientific interest.

DEFINITION. (FUNCTION) . *A function from set X to set Y is a relation $F \subseteq X \times Y$, that associates to $x \in X$ a single $y \in Y$.*

The above intuitive definition can be transcribed in precise mathematical terms as $F \subseteq X \times Y$ is a *function* if $(x,y) \in F$ and $(x,z) \in F$ implies $y = z$. Since it's a particular kind of relation, a function is a triplet of sets (X, Y, F), but with a special, common notation to denote the triplet by $f : X \longrightarrow Y$, with $F = \{(x, f(x)) \mid x \in X, f(x) \in Y\}$ and the property that $(x,y) \in F \Longrightarrow y = f(x)$. The set X is the *domain* and the set Y is the *codomain* of the function f. The value from the domain $x \in X$ is the *argument* of the function associated with the *function value* $y = f(x)$. The function value y is said to be *returned* by evaluation $y = f(x)$. The previously defined relations R, P, I are functions but $S = \{(a,\alpha),(a,\beta),(a,\gamma)\}$ is not. All relations can be inverted, and inversion of a function defines a new relation, but which might not itself be a function. For example the relation $S^{-1} = \{(\alpha,a),(\beta,a),(\gamma,a)\}$ is a function, but its inverse $(S^{-1})^{-1} = S$ is not.

Familiar functions include:

- the trigonometric functions $\cos : \mathbb{R} \longrightarrow [-1,1]$, $\sin : \mathbb{R} \longrightarrow [-1,1]$ that for argument $\theta \in \mathbb{R}$ return the function values $\cos(\theta), \sin(\theta)$ giving the Cartesian coordinates $(x,y) \in \mathbb{R}^2$ of a point on the unit circle at angular extent θ from the x-axis;
- the exponential and logarithm functions $\exp : \mathbb{R} \longrightarrow \mathbb{R}$, $\log : (0,\infty) \longrightarrow \mathbb{R}$, as well as power and logarithm functions in some other base a;
- polynomial functions $p_n : \mathbb{R} \longrightarrow \mathbb{R}$, defined by a succession of additions and multiplications

$$p_n(x) = a_n x^n + a_{n-1} x^{n-1} + \cdots + a_1 x + a_0 = \sum_{i=0}^{n} a_i x^i = ((a_n x + a_{n-1})x + \cdots + a_1)x + a_0.$$

Simple functions such as sin, cos, exp, log, are predefined in Octave, and when given a vector argument return the function applied to each vector component.

```
octave] disp(cos(0:pi/4:pi))
   1.0000e+00   7.0711e-01   6.1232e-17  -7.0711e-01  -1.0000e+00
octave] y=log2(1:8); disp(y)
   0.00000   1.00000   1.58496   2.00000   2.32193   2.58496   2.80735   3.00000
octave] disp(pow2(y))
   1.0000   2.0000   3.0000   4.0000   5.0000   6.0000   7.0000   8.0000
octave] a=[1 0 -1]; x=-2:2; y=polyval(a,x); disp(y)
   3   0  -1   0   3
octave]
```

As seen previously, a Euclidean space $E_m = (\mathbb{R}^m, \mathbb{R}, +, \cdot)$ can be used to suggest properties of more complex spaces such as the vector space of continuous functions $C^0(\mathbb{R})$. A construct that will be often used is to interpret a vector within E_m as a function, since $v \in \mathbb{R}^m$ with components $v = [\ v_1\ \ v_2\ \ \ldots\ \ v_m\ ]^T$ also defines a function $v : \{1,2,\ldots,m\} \longrightarrow \mathbb{R}$, with values $v(i) = v_i$. As the number of components grows the function v can provide better approximations of some continuous function $f \in C^0(\mathbb{R})$ through the function values $v_i = v(i) = f(x_i)$ at distinct sample points $x_1, x_2, \ldots, x_m$.

The above function examples are all defined on a domain of scalars or naturals and returned scalar values. Within linear algebra the particular interest is on functions defined on sets of vectors from some vector space $\mathcal{V} = (V, S, +, \cdot)$ that return either scalars $f: V \longrightarrow S$, or vectors from some other vector space $\mathcal{W} = (W, S, +, \cdot)$, $\boldsymbol{g}: V \longrightarrow W$. The codomain of a vector-valued function might be the same set of vectors as its domain, $\boldsymbol{h}: V \longrightarrow V$. The fundamental operation within linear algebra is the linear combination $a\boldsymbol{u} + b\boldsymbol{v}$ with $a, b \in S$, $\boldsymbol{u}, \boldsymbol{v} \in V$. A key aspect is to characterize how a function behaves when given a linear combination as its argument, for instance $f(a\boldsymbol{u} + b\boldsymbol{v})$ or $\boldsymbol{g}(a\boldsymbol{u} + b\boldsymbol{v})$.

1.3. Linear functionals

Consider first the case of a function defined on a set of vectors that returns a scalar value. These can be interpreted as labels attached to a vector, and are very often encountered in applications from natural phenomena or data analysis.

DEFINITION. (FUNCTIONAL) . *A functional on vector space $\mathcal{V} = (V, S, +, \cdot)$ is a function from the set of vectors V to the set of scalars S of the vector space $\mathcal{V}$.*

DEFINITION. (LINEAR FUNCTIONAL) . *The functional $f: V \longrightarrow S$ on vector space $\mathcal{V} = (V, S, +, \cdot)$ is a linear functional if for any two vectors $\boldsymbol{u}, \boldsymbol{v} \in V$ and any two scalars a, b*

$$f(a\boldsymbol{u} + b\boldsymbol{v}) = af(\boldsymbol{u}) + bf(\boldsymbol{v}). \tag{1.5}$$

Many different functionals may be defined on a vector space $\mathcal{V} = (V, S, +, \cdot)$, and an insightful alternative description is provided by considering the set of all linear functionals, that will be denoted as $V^* = \{f \mid f: V \longrightarrow S\}$. These can be organized into another vector space $\mathcal{V}^* = (V^*, S, +, \cdot)$ with vector addition of linear functionals $f, g \in V^*$ and scaling by $a \in S$ defined by

$$(f + g)(\boldsymbol{u}) = f(\boldsymbol{u}) + g(\boldsymbol{u}), (af)(\boldsymbol{u}) = af(\boldsymbol{u}), \boldsymbol{u} \in V. \tag{1.6}$$

DEFINITION. (DUAL VECTOR SPACE) . *For some vector space $\mathcal{V}$, the vector space of linear functionals $\mathcal{V}^*$ is called the dual vector space.*

As is often the case, the above abstract definition can better be understood by reference to the familiar case of Euclidean space. Consider $\mathcal{R}_2 = (\mathbb{R}^2, \mathbb{R}, +, \cdot)$, the set of vectors in the plane with $\boldsymbol{x} \in \mathbb{R}^2$ the position vector from the origin $(0, 0)$ to point X in the plane with coordinates (x_1, x_2). One functional from the dual space $\mathcal{R}_2^*$ is $f_2(\boldsymbol{x}) = x_2$, i.e., taking the second coordinate of the position vector. The linearity property is readily verified. For $\boldsymbol{x}, \boldsymbol{y} \in \mathcal{R}_2$, $a, b \in \mathbb{R}$,

$$f_2(a\boldsymbol{x} + b\boldsymbol{y}) = ax_2 + by_2 = af_2(\boldsymbol{x}) + bf_2(\boldsymbol{y}).$$

Given some constant value $h \in \mathbb{R}$, the curves within the plane defined by $f_2(\boldsymbol{x}) = h$ are called the *contour lines* or *level sets* of f_2. Several contour lines and position vectors are shown in Figure 1.4. The utility of functionals and dual spaces can be shown by considering a simple example from physics. Assume that x_2 is the height above ground level and a vector $\boldsymbol{x}$ is the displacement of a body of mass m in a gravitational field. The mechanical work done to lift the body from ground level to height h is $W = mgh$ with g the gravitational acceleration. The mechanical work is the same for all displacements $\boldsymbol{x}$ that satisfy the equation $f_2(\boldsymbol{x}) = h$. The work expressed in units $mg\Delta h$ can be interpreted as the number of contour lines $f_2(\boldsymbol{x}) = n\Delta h$ intersected by the displacement vector $\boldsymbol{x}$. This concept of duality between vectors and scalar-valued functionals arises throughout mathematics, the physical and social sciences and in data science. The term "duality" itself comes from geometry. A point X in $\mathbb{R}^2$ with coordinates (x_1, x_2) can be defined either as the end-point of the position vector $\boldsymbol{x}$, or as the intersection of the contour lines of two funtionals $f_1(\boldsymbol{x}) = x_1$ and $f_2(\boldsymbol{x}) = x_2$. Either geometric description works equally well in specifying the position of X, so it might seem redundant to have two such procedures. It turns out though that many quantities of interest in applications can be defined through use of both descriptions, as shown in the computation of mechanical work in a gravitational field.

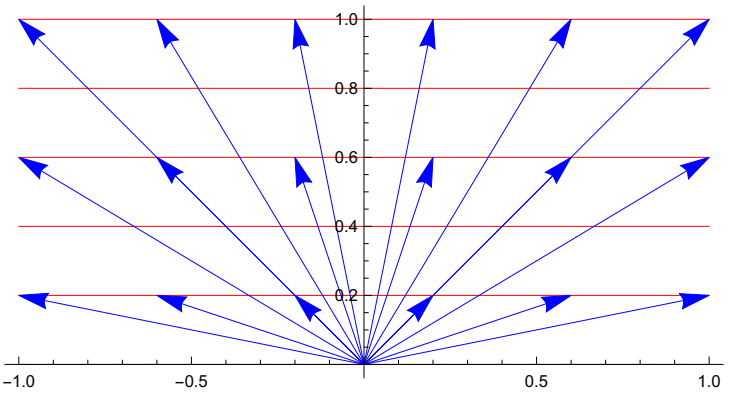


Figure 1.4. Vectors in E_2 and contour lines of the functional $f(\boldsymbol{x}) = x_2$

1.4. Linear mappings

Consider now functions $\boldsymbol{f}: V \longrightarrow W$ from vector space $\mathcal{V} = (V, S, +, \cdot)$ to another vector space $\mathcal{W} = (W, T, +, \cdot)$. As before, the action of such functions on linear combinations is of special interest.

DEFINITION. (LINEAR MAPPING) . *A function $\boldsymbol{f}: V \longrightarrow W$, from vector space $\mathcal{V} = (V, S, +, \cdot)$ to vector space $\mathcal{W} = (W, S, \oplus, \odot)$ is called a linear mapping if for any two vectors $\boldsymbol{u}, \boldsymbol{v} \in V$ and any two scalars $a, b \in S$*

$$\boldsymbol{f}(a\boldsymbol{u} + b\boldsymbol{v}) = a\boldsymbol{f}(\boldsymbol{u}) + b\boldsymbol{f}(\boldsymbol{v}). \tag{1.7}$$

The image of a linear combination $a\boldsymbol{u} + b\boldsymbol{v}$ through a linear mapping is another linear combination $a\boldsymbol{f}(\boldsymbol{u}) + b\boldsymbol{f}(\boldsymbol{v})$, and linear mappings are said to preserve the structure of a vector space, and called *homomorphisms* in mathematics. The codomain of a linear mapping might be the same as the domain in which case the mapping is said to be an *endomorphism*.

Matrix-vector multiplication has been introduced as a concise way to specify a linear combination

$$\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x} = x_1\boldsymbol{a}_1 + \cdots + x_n\boldsymbol{a}_n,$$

with $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_n$ the columns of the matrix, $\boldsymbol{A} = [\ \boldsymbol{a}_1\ \ \boldsymbol{a}_2\ \ \ldots\ \ \boldsymbol{a}_n\ ]$. This is a linear mapping between the real spaces $\mathcal{R}_m$, $\mathcal{R}_n$, $\boldsymbol{f}: \mathbb{R}^m \longrightarrow \mathbb{R}^n$, and indeed any linear mapping between real spaces can be given as a matrix-vector product.

2. Measurements

Vectors within the real space $\mathcal{R}_m$ can be completely specified by m real numbers, even though m is large in many realistic applications. A vector within $C^0(\mathbb{R})$, i.e., a continuous function defined on the reals, cannot be so specified since it would require an infinite, non-countable listing of function values. In either case, the task of describing the elements of a vector space $\mathcal{V} = (V, S, +, \cdot)$ by simpler means arises. Within data science this leads to *classification problems* in accordance with some relevant criteria.

2.1. Equivalence classes

Many classification criteria are scalars, defined as a scalar-valued function $f: \mathcal{V} \longrightarrow S$ on a vector space, $\mathcal{V} = (V, S, +, \cdot)$. The most common criteria are inspired by experience with Euclidean space. In a Euclidean-Cartesian model $(\mathbb{R}^2, \mathbb{R}, +, \cdot)$ of the geometry of a plane Π, a point $O \in \Pi$ is arbitrarily chosen to correspond to the zero vector $\boldsymbol{0} = [\ 0\ \ 0\ ]^T$, along with two preferred vectors $\boldsymbol{e}_1, \boldsymbol{e}_2$ grouped together into the identity matrix $\boldsymbol{I}$. The position of a point $X \in \Pi$ with respect to O is given by the linear combination

$$\boldsymbol{x} = \boldsymbol{I}\boldsymbol{x} + \boldsymbol{0} = [\ \boldsymbol{e}_1\ \ \boldsymbol{e}_2\ ] \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = x_1\boldsymbol{e}_1 + x_2\boldsymbol{e}_2\,.$$

Several possible classifications of points in the plane are depicted in Figure 1.5: lines, squares, circles. Intuitively, each choice separates the plane into subsets, and a given point in the plane belongs to just one in the chosen family of subsets. A more precise characterization is given by the concept of a partition of a set.

DEFINITION. (PARTITION) . *A partition of a set is a grouping of its elements into non-empty subsets such that every element is included in exactly one subset.*

In precise mathematical terms, a partition of set S is $P=\{S_i \mid S_i \subset P, S_i \neq \emptyset, i \in I\}$ such that $\forall x \in S, \exists! j \in I$ for which $x \in S_j$. Since there is only one set ($\exists!$ signifies "exists and is unique") to which some given $x \in S$ belongs, the subsets S_i of the partition P are disjoint, $i \neq j \Longrightarrow S_i \cap S_j = \emptyset$. The subsets S_i are labeled by i within some index set I. The index set might be a subset of the naturals, $I \subset \mathbb{N}$ in which case the partition is countable, possibly finite. The partitions of the plane suggested by Figure 1.5 are however indexed by a real-valued label, $i \in \mathbb{R}$ with $I \subset \mathbb{R}$.

A technique which is often used to generate a partition of a vector space $\mathcal{V}=(V,S,+,\cdot)$ is to define an equivalence relation between vectors, $H \subseteq V \times V$. For some element $\boldsymbol{u} \in V$, the *equivalence class* of $\boldsymbol{u}$ is defined as all vectors $\boldsymbol{v}$ that are equivalent to $\boldsymbol{u}$, $\{\boldsymbol{v} \mid (\boldsymbol{u},\boldsymbol{v}) \in H\}$. The set of equivalence classes of is called the *quotient set* and denoted as V/H, and the quotient set is a partition of V. Figure 1.5 depicts four different partitions of the plane. These can be interpreted geometrically, such as parallel lines or distance from the origin. With wider implications for linear algebra, the partitions can also be given in terms of classification criteria specified by functions.

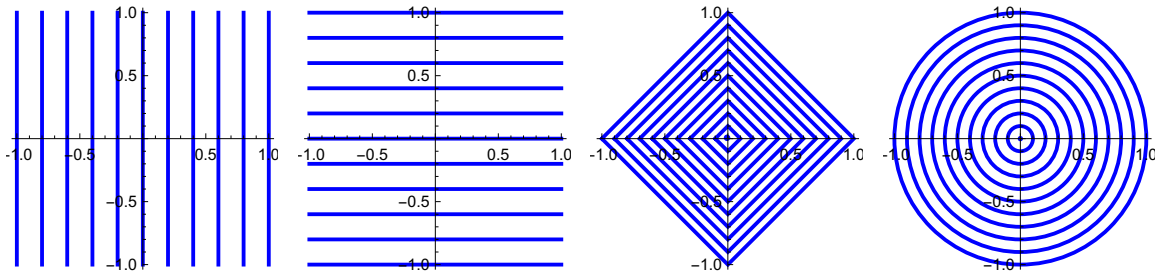


Figure 1.5. Equivalence classes within the plane

2.2. Norms

The partition of $\mathbb{R}^2$ by circles from Figure 1.5 is familiar; the equivalence classes are sets of points whose position vector has the same size, $\{\boldsymbol{x}=\begin{bmatrix} x_1 & x_2 \end{bmatrix}^T \mid (x_1^2+x_2^2)^{1/2}=r\}$, or is at the same distance from the origin. Note that familiarity with Euclidean geometry should not obscure the fact that some other concept of distance might be induced by the data. A simple example is statement of walking distance in terms of city blocks, in which the distance from a starting point to an address $x_1=3$ blocks east and $x_2=4$ blocks north is $x_1+x_2=7$ city blocks, not the Euclidean distance $(x_1^2+x_2^2)^{1/2}=5$ since one cannot walk through the buildings occupying a city block.

The above observations lead to the mathematical concept of a *norm* as a tool to evaluate vector magnitude. Recall that a vector space is specified by two sets and two operations, $\mathcal{V}=(V,S,+,\cdot)$, and the behavior of a norm with respect to each of these components must be defined. The desired behavior includes the following properties and formal definition.

Unique value. The magnitude of a vector $\boldsymbol{v} \in V$ should be a unique scalar, requiring the definition of a function. The scalar could have irrational values and should allow ordering of vectors by size, so the function should be from V to $\mathbb{R}$, $f: V \longrightarrow \mathbb{R}$. On the real line the point at coordinate x is at distance $|x|$ from the origin, and to mimic this usage the norm of $\boldsymbol{v} \in V$ is denoted as $\|\boldsymbol{v}\|$, leading to the definition of a function $\| \ \|: V \longrightarrow \mathbb{R}_+$, $\mathbb{R}_+ = \{a \mid a \in \mathbb{R}, a \geq 0\}$.

Null vector case. Provision must be made for the only distinguished element of V, the null vector $\boldsymbol{0}$. It is natural to associate the null vector with the null scalar element, $\|\boldsymbol{0}\|=0$. A crucial additional property is also imposed namely that the null vector is the *only* vector whose norm is zero, $\|\boldsymbol{v}\|=0 \Longrightarrow \boldsymbol{v}=\boldsymbol{0}$. From knowledge of a single scalar value, an entire vector can be determined. This property arises at key junctures in linear algebra, notably in providing a link to another branch of mathematics known as analysis, and is needed to establish the fundamental theorem of linear algbera or the singular value decomposition encountered later.

Scaling. Transfer of the scaling operation $\boldsymbol{v} = a\boldsymbol{u}$ property leads to imposing $\|\boldsymbol{v}\| = |a|\,\|\boldsymbol{u}\|$. This property ensures commensurability of vectors, meaning that the magnitude of vector $\boldsymbol{v}$ can be expressed as a multiple of some standard vector magnitude $\|\boldsymbol{u}\|$.

Vector addition. Position vectors from the origin to coordinates $x, y > 0$ on the real line can be added and $|x+y| = |x| + |y|$. If however the position vectors point in different directions, $x > 0$, $y < 0$, then $|x+y| < |x| + |y|$. For a general vector space the analogous property is known as the *triangle inequality*, $\|\boldsymbol{u}+\boldsymbol{v}\| \leqslant \|\boldsymbol{u}\| + \|\boldsymbol{v}\|$ for $\boldsymbol{u}, \boldsymbol{v} \in V$.

DEFINITION. (NORM) . *A norm on the vector space $\mathcal{V} = (V, S, +, \cdot)$ is a function $\|\ \| : V \longrightarrow \mathbb{R}_+$ that for $\boldsymbol{u}, \boldsymbol{v} \in V$, $a \in S$ satisfies:*

1. $\|\boldsymbol{v}\| = 0 \Longrightarrow \boldsymbol{v} = \boldsymbol{0}$;
2. $\|a\boldsymbol{u}\| = |a|\,\|\boldsymbol{u}\|$;
3. $\|\boldsymbol{u}+\boldsymbol{v}\| \leqslant \|\boldsymbol{u}\| + \|\boldsymbol{v}\|$.

Note that the norm is a functional, but the triangle inequality implies that it is not generally a linear functional. Returning to Figure 1.5, consider the functions $f_i : \mathbb{R}^2 \longrightarrow \mathbb{R}_+$ defined for $\boldsymbol{x} = [\ x_1\ \ x_2\ ]^T$ through values

$$f_1(\boldsymbol{x}) = |x_1|\,, f_2(\boldsymbol{x}) = |x_2|\,, f_3(\boldsymbol{x}) = |x_1| + |x_2|\,, f_4(\boldsymbol{x}) = (|x_1|^2 + |x_2|^2)^{1/2}.$$

Sets of constant value of the above functions are also equivalence classes induced by the equivalence relations E_i for $i = 1, 2, 3, 4$.

1. $f_1(\boldsymbol{x}) = c \Longrightarrow |x_1| = c$, $E_1 = \{(\boldsymbol{x}, \boldsymbol{y}) \mid f_1(\boldsymbol{x}) = f_1(\boldsymbol{y}) \Longleftrightarrow |x_1| = |y_1|\ \} \subseteq \mathbb{R}^2 \times \mathbb{R}^2$;
2. $f_2(\boldsymbol{x}) = c \Longrightarrow |x_2| = c$, $E_2 = \{(\boldsymbol{x}, \boldsymbol{y}) \mid f_2(\boldsymbol{x}) = f_2(\boldsymbol{y}) \Longleftrightarrow |x_2| = |y_2|\ \} \subseteq \mathbb{R}^2 \times \mathbb{R}^2$;
3. $f_3(\boldsymbol{x}) = c \Longrightarrow |x_1| + |x_2| = c$, $E_3 = \{(\boldsymbol{x}, \boldsymbol{y}) \mid f_3(\boldsymbol{x}) = f_3(\boldsymbol{y}) \Longleftrightarrow |x_1| + |x_2| = |y_1| + |y_2|\ \} \subseteq \mathbb{R}^2 \times \mathbb{R}^2$;
4. $f_4(\boldsymbol{x}) = c \Longrightarrow (|x_1|^2 + |x_2|^2)^{1/2} = c$, $E_4 = \{(\boldsymbol{x}, \boldsymbol{y}) \mid f_4(\boldsymbol{x}) = f_4(\boldsymbol{y}) \Longleftrightarrow (|x_1|^2 + |x_2|^2)^{1/2} = (|y_1|^2 + |y_2|^2)^{1/2}\} \subseteq \mathbb{R}^2 \times \mathbb{R}^2$.

These equivalence classes correspond to the vertical lines, horizontal lines, squares, and circles of Figure 1.5. Not all of the functions f_i are norms since $f_1(\boldsymbol{x})$ is zero for the non-null vector $\boldsymbol{x} = [\ 0\ \ 1\ ]^T$, and $f_2(\boldsymbol{x})$is zero for the non-null vector $\boldsymbol{x} = [\ 1\ \ 0\ ]^T$. The functions f_3 and f_4 are indeed norms, and specific cases of the following general norm.

DEFINITION. (p-NORM IN $\mathcal{R}_m$) . *The p-norm on the real vector space $\mathcal{R}_m = (\mathbb{R}^m, \mathbb{R}, +, \cdot)$ for $p \geqslant 1$ is the function $\|\ \|_p$: $V \longrightarrow \mathbb{R}_+$ with values $\|\boldsymbol{x}\|_p = (|x_1|^p + |x_2|^p + \cdots + |x_m|^p)^{1/p}$, or*

$$\|\boldsymbol{x}\|_p = \left(\sum_{i=1}^{m} |x_i|^p \right)^{1/p} \text{ for } \boldsymbol{x} \in \mathbb{R}^m. \tag{1.8}$$

Denote by x_i the largest component in absolute value of $\boldsymbol{x} \in \mathbb{R}^m$. As p increases, $|x_i|^p$ becomes dominant with respect to all other terms in the sum suggesting the definition of an inf-norm by

$$\|\boldsymbol{x}\|_\infty = \max_{1 \leqslant i \leqslant m} |x_i|\,.$$

This also works for vectors with equal components, since the fact that the number of components is finite while $p \longrightarrow \infty$ can be used as exemplified for $\boldsymbol{x} = [\ a\ \ a\ \ \ldots\ \ a\ ]^T$, by $\|\boldsymbol{x}\|_p = (m\,|a|^p)^{1/p} = m^{1/p}\,|a|$, with $m^{1/p} \longrightarrow 1$.

Note that the Euclidean norm corresponds to $p = 2$, and is often called the 2-norm. The analogy between vectors and functions can be exploited to also define a p-norm for $\mathcal{C}^0[a,b] = (C([a,b]), \mathbb{R}, +, \cdot)$, the vector space of continuous functions defined on $[a, b]$.

DEFINITION. (p-NORM IN $\mathcal{C}^0[a,b]$) . *The p-norm on the vector space of continuous functions $\mathcal{C}^0[a,b]$ for $p \geqslant 1$ is the function $\|\ \|_p$: $V \longrightarrow \mathbb{R}_+$ with values*

$$\|f\|_p = \left(\int_a^b |f(x)|^p \,\mathrm{d}x \right)^{1/p}, \text{for } f \in C[a,b]. \tag{1.9}$$

The integration operation $\int_a^b$ can be intuitively interpreted as the value of the sum $\sum_{i=1}^m$ from equation (1.8) for very large m and very closely spaced evaluation points of the function $f(x_i)$, for instance $|x_{i+1}-x_i| = (b-a)/m$. An inf-norm can also be define for continuous functions by

$$\|f\|_\infty = \sup_{x\in[a,b]} |f(x)|,$$

where sup, the supremum operation can be intuitively understood as the generalization of the max operation over the countable set $\{1,2,\ldots,m\}$ to the uncountable set $[a,b]$.

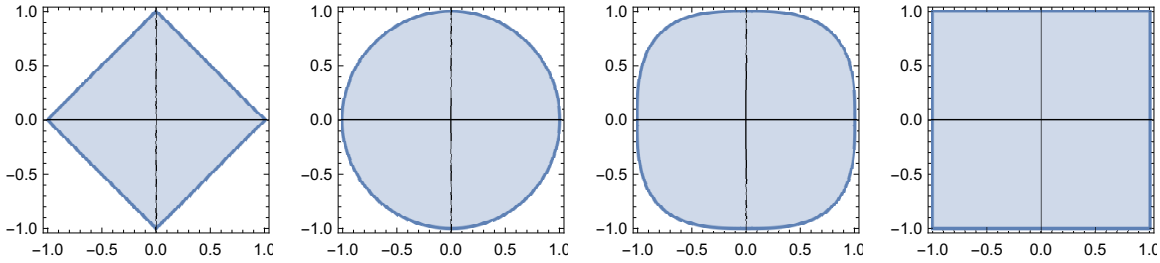


Figure 1.6. Regions within $\mathbb{R}^2$ for which $\|\boldsymbol{x}\|_p \leq 1$, for $p = 1, 2, 3, \infty$.

Vector norms arise very often in applications, especially in data science since they can be used to classify data, and are implemented in software systems such as Octave in which the `norm` function with a single argument computes the most commonly encountered norm, the 2-norm. If a second argument p is specified the p-norm is computed.

```
octave] x=[1; 1; 1]; disp([norm(x) sqrt(3)])
   1.7321   1.7321
octave] m=9; x=ones(m,1); disp([norm(x) sqrt(m)])
   3   3
octave] m=4; x=ones(m,1); disp([norm(x,1) m])
   4   4
octave] disp([norm(x,1) norm(x,2) norm(x,4) norm(x,8) norm(x,16) norm(x,inf)])
   4.0000   2.0000   1.4142   1.1892   1.0905   1.0000
octave]
```

2.3. Inner product

Norms are functionals that define what is meant by the size of a vector, but are not linear. Even in the simplest case of the real line, the linearity relation $|x+y| = |x| + |y|$ is not verified for $x>0$, $y<0$. Nor do norms characterize the familiar geometric concept of orientation of a vector. A particularly important orientation from Euclidean geometry is orthogonality between two vectors. Another function is required, but before a formal definition some intuitive understanding is sought by considering vectors and functionals in the plane, as depicted in Figure 1.7. Consider a position vector $\boldsymbol{x} = [\ x_1\ \ x_2\ ]^T \in \mathbb{R}^2$ and the previously-encountered linear functionals

$$f_1, f_2 : \mathbb{R}^2 \longrightarrow \mathbb{R},\ f_1(\boldsymbol{x}) = x_1,\ f_2(\boldsymbol{x}) = x_2.$$

The x_1 component of the vector $\boldsymbol{x}$ can be thought of as the number of level sets of f_1 times it crosses; similarly for the x_2 component. A convenient labeling of level sets is by their normal vectors. The level sets of f_1 have normal $\boldsymbol{e}_1^T = [\ 1\ \ 0\ ]$, and those of f_2 have normal vector $\boldsymbol{e}_2^T = [\ 0\ \ 1\ ]$. Both of these can be thought of as matrices with two columns, each containing a single component. The products of these matrices with the vector $\boldsymbol{x}$ gives the value of the functionals f_1, f_2

$$\boldsymbol{e}_1^T\boldsymbol{x} = [\ 1\ \ 0\ ]\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = 1\cdot x_1 + 0\cdot x_2 = x_1 = f_1(\boldsymbol{x}),$$

$$\boldsymbol{e}_2^T\boldsymbol{x} = [\ 0\ \ 1\ ]\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = 0\cdot x_1 + 1\cdot x_2 = x_1 = f_2(\boldsymbol{x}).$$

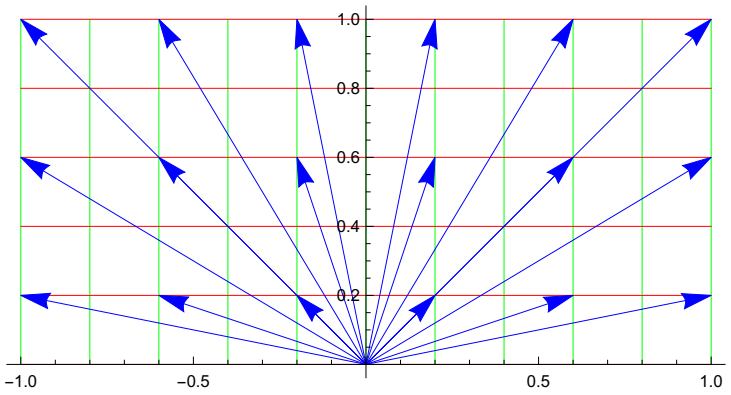


Figure 1.7. Euclidean space E_2 and its dual E_2^*.

In general, any linear functional f defined on the real space $\mathscr{R}_m$ can be labeled by a vector

$$\boldsymbol{a}^T = [\ a_1\ \ a_2\ \ \ldots\ \ a_m\ ],$$

and evaluated through the matrix-vector product $f(\boldsymbol{x}) = \boldsymbol{a}^T\boldsymbol{x}$. This suggests the definition of another function s: $\mathbb{R}^m \times \mathbb{R}^m \longrightarrow \mathbb{R}$,

$$s(\boldsymbol{a}, \boldsymbol{x}) = \boldsymbol{a}^T\boldsymbol{x}.$$

The function s is called an *inner product*, has two vector arguments from which a matrix-vector product is formed and returns a scalar value, hence is also called a *scalar product*. The definition from an Euclidean space can be extended to general vector spaces. For now, consider the field of scalars to be the reals $S = \mathbb{R}$.

DEFINITION. (INNER PRODUCT) . *An inner product in the vector space $\mathcal{U} = (V, \mathbb{R}, +, \cdot)$ is a function s: $V \times V \longrightarrow \mathbb{R}$ with properties*

Symmetry. *For any $\boldsymbol{a}, \boldsymbol{x} \in V$, $s(\boldsymbol{a}, \boldsymbol{x}) = s(\boldsymbol{x}, \boldsymbol{a})$.*

Linearity in second argument. *For any $\boldsymbol{a}, \boldsymbol{x}, \boldsymbol{y} \in V$, $\alpha, \beta \in \mathbb{R}$, $s(\boldsymbol{a}, \alpha\boldsymbol{x} + \beta\boldsymbol{y}) = \alpha s(\boldsymbol{a}, \boldsymbol{x}) + \beta s(\boldsymbol{a}, \boldsymbol{y})$.*

Positive definiteness. *For any $\boldsymbol{x} \in V \backslash \{\boldsymbol{0}\}$, $s(\boldsymbol{x}, \boldsymbol{x}) > 0$.*

The inner product $s(\boldsymbol{a}, \boldsymbol{x})$ returns the number of level sets of the functional labeled by $\boldsymbol{a}$ crossed by the vector $\boldsymbol{x}$, and this interpretation underlies many applications in the sciences as in the gravitational field example above. Inner products also provide a procedure to evaluate geometrical quantities and relationships.

Vector norm. In $\mathscr{R}_m$ the number of level sets of the functional labeled by $\boldsymbol{x}$ crossed by $\boldsymbol{x}$ itself is identical to the square of the 2-norm

$$s(\boldsymbol{x}, \boldsymbol{x}) = \boldsymbol{x}^T\boldsymbol{x} = \| \boldsymbol{x} \|_2^2.$$

In general, the square root of $s(\boldsymbol{x}, \boldsymbol{x})$ satisfies the properties of a norm, and is called the norm induced by an inner product

$$\| \boldsymbol{x} \| = s(\boldsymbol{x}, \boldsymbol{x})^{1/2}.$$

A real space together with the scalar product $s(\boldsymbol{x}, \boldsymbol{y}) = \boldsymbol{x}^T\boldsymbol{y}$ and induced norm $\| \boldsymbol{x} \| = s(\boldsymbol{x}, \boldsymbol{x})^{1/2}$ defines an Euclidean vector space $\mathscr{E}_m$.

Orientation. In $\mathscr{E}_2$ the point specified by polar coordinates (r, θ) has the Cartesian coordinates $x_1 = r\cos\theta$, $x_2 = r\sin\theta$, and position vector $\boldsymbol{x} = [\ x_1\ \ x_2\ ]^T$. The inner product

$$\boldsymbol{e}_1^T\boldsymbol{x} = [\ 1\ \ 0\ ]\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = 1 \cdot x_1 + 0 \cdot x_2 = r\cos\theta,$$

is seen to contain information on the relative orientation of $\boldsymbol{x}$ with respect to $\boldsymbol{e}_1$. In general, the angle θ between two vectors $\boldsymbol{x}, \boldsymbol{y}$ with any vector space with a scalar product can be defined by

$$\cos\theta = \frac{s(\boldsymbol{x}, \boldsymbol{y})}{[s(\boldsymbol{x}, \boldsymbol{x})\, s(\boldsymbol{y}, \boldsymbol{y})]^{1/2}} = \frac{s(\boldsymbol{x}, \boldsymbol{y})}{\| \boldsymbol{x} \|\ \| \boldsymbol{y} \|},$$

which becomes

$$\cos\theta = \frac{\boldsymbol{x}^T\boldsymbol{y}}{\|\boldsymbol{x}\|\,\|\boldsymbol{y}\|},$$

in a Euclidean space, $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^m$.

Orthogonality. In $\mathscr{E}_2$ two vectors are orthogonal if the angle between them is such that $\cos\theta = 0$, and this can be extended to an arbitrary vector space $\mathscr{V} = (V, \mathbb{R}, +, \cdot)$ with a scalar product by stating that $\boldsymbol{x}, \boldsymbol{y} \in V$ are orthogonal if $s(\boldsymbol{x}, \boldsymbol{y}) = 0$. In $\mathscr{E}_m$ vectors $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^m$ are orthogonal if $\boldsymbol{x}^T\boldsymbol{y} = 0$.

3. Linear mapping composition

3.1. Matrix-matrix product

From two functions $f: A \longrightarrow B$ and $g: B \longrightarrow C$, a composite function, $h = g \circ f$, $h: A \longrightarrow C$ is defined by

$$h(x) = g(f(x)).$$

Consider linear mappings between Euclidean spaces $\boldsymbol{f}: \mathbb{R}^n \longrightarrow \mathbb{R}^m$, $\boldsymbol{g}: \mathbb{R}^m \longrightarrow \mathbb{R}^p$. Recall that linear mappings between Euclidean spaces are expressed as matrix vector multiplication

$$\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x}, \boldsymbol{g}(\boldsymbol{y}) = \boldsymbol{B}\boldsymbol{y}, \boldsymbol{A} \in \mathbb{R}^{m\times n}, \boldsymbol{B} \in \mathbb{R}^{p\times m}.$$

The composite function $\boldsymbol{h} = \boldsymbol{g} \circ \boldsymbol{f}$ is $\boldsymbol{h}: \mathbb{R}^n \longrightarrow \mathbb{R}^p$, defined by

$$\boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{g}(\boldsymbol{f}(\boldsymbol{x})) = \boldsymbol{g}(\boldsymbol{A}\boldsymbol{x}) = \boldsymbol{B}\boldsymbol{A}\boldsymbol{x}.$$

Note that the intemediate vector $\boldsymbol{u} = \boldsymbol{A}\boldsymbol{x}$ is subsequently multiplied by the matrix $\boldsymbol{B}$. The composite function $\boldsymbol{h}$ is itself a linear mapping

$$\boldsymbol{h}(a\boldsymbol{x} + b\boldsymbol{y}) = \boldsymbol{B}\boldsymbol{A}(a\boldsymbol{x} + b\boldsymbol{y}) = \boldsymbol{B}\,(a\boldsymbol{A}\boldsymbol{x} + b\boldsymbol{A}\boldsymbol{y}) = \boldsymbol{B}(a\boldsymbol{u} + b\boldsymbol{v}) = a\boldsymbol{B}\boldsymbol{u} + b\boldsymbol{B}\boldsymbol{v} = a\boldsymbol{B}\boldsymbol{A}\boldsymbol{x} + b\boldsymbol{B}\boldsymbol{A}\boldsymbol{y} = a\boldsymbol{h}(\boldsymbol{x}) + b\boldsymbol{h}(\boldsymbol{y}),$$

so it also can be expressed a matrix-vector multiplication

$$\boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{C}\boldsymbol{x} = \boldsymbol{B}\boldsymbol{A}\boldsymbol{x}. \tag{1.10}$$

Using the above, $\boldsymbol{C}$ is defined as the product of matrix $\boldsymbol{B}$ with matrix $\boldsymbol{A}$

$$\boldsymbol{C} = \boldsymbol{B}\boldsymbol{A}.$$

The columns of $\boldsymbol{C}$ can be determined from those of $\boldsymbol{A}$ by considering the action of $\boldsymbol{h}$ on the the column vectors of the identity matrix $\boldsymbol{I} = [\ \boldsymbol{e}_1\ \ \boldsymbol{e}_2\ \ \dots\ \ \boldsymbol{e}_n\ ] \in \mathbb{R}^{n\times n}$. First, note that

$$\boldsymbol{A}\boldsymbol{e}_j = [\ \boldsymbol{a}_1\ \ \boldsymbol{a}_2\ \ \dots\ \ \boldsymbol{a}_n\ ] \begin{bmatrix} 1 \\ 0 \\ \vdots \\ \vdots \\ 0 \end{bmatrix} = \boldsymbol{a}_1, \dots, \boldsymbol{A}\boldsymbol{e}_j = [\ \boldsymbol{a}_1\ \ \boldsymbol{a}_2\ \ \dots\ \ \boldsymbol{a}_n\ ] \begin{bmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix} = \boldsymbol{a}_j, \boldsymbol{A}\boldsymbol{e}_n = [\ \boldsymbol{a}_1\ \ \boldsymbol{a}_2\ \ \dots\ \ \boldsymbol{a}_n\ ] \begin{bmatrix} 0 \\ \vdots \\ \vdots \\ 0 \\ 1 \end{bmatrix} = \boldsymbol{a}_n. \tag{1.11}$$

The above can be repeated for the matrix $\boldsymbol{C} = [\ \boldsymbol{c}_1\ \ \boldsymbol{c}_2\ \ \dots\ \ \boldsymbol{c}_n\ ]$ giving

$$\boldsymbol{h}(\boldsymbol{e}_1) = \boldsymbol{C}\boldsymbol{e}_1 = \boldsymbol{c}_1, \dots, \boldsymbol{h}(\boldsymbol{e}_j) = \boldsymbol{C}\boldsymbol{e}_j = \boldsymbol{c}_j, \dots, \boldsymbol{h}(\boldsymbol{e}_n) = \boldsymbol{C}\boldsymbol{e}_n = \boldsymbol{c}_n. \tag{1.12}$$

Combining the above equations leads to $\boldsymbol{c}_j = \boldsymbol{B}\boldsymbol{a}_j$, or

$$\boldsymbol{C} = [\ \boldsymbol{c}_1\ \ \boldsymbol{c}_2\ \ \dots\ \ \boldsymbol{c}_n\ ] = \boldsymbol{B}\,[\ \boldsymbol{a}_1\ \ \boldsymbol{a}_2\ \ \dots\ \ \boldsymbol{a}_n\ ].$$

From the above the matrix-matrix product $\boldsymbol{C} = \boldsymbol{B}\boldsymbol{A}$ is seen to simply be a grouping of all the products of $\boldsymbol{B}$ with the column vectors of $\boldsymbol{A}$,

$$\boldsymbol{C} = [\ \boldsymbol{c}_1\ \ \boldsymbol{c}_2\ \ \dots\ \ \boldsymbol{c}_n\ ] = [\boldsymbol{B}\ \boldsymbol{a}_1\ \ \boldsymbol{B}\boldsymbol{a}_2\ \ \dots\ \ \boldsymbol{B}\boldsymbol{a}_n\ ]$$

Matrix-vector and matrix-matrix products are implemented in Octave, the above results can readily be verified.

```
octave] a1=[1; 2]; a2=[3; 4]; A=[a1 a2]
A =

   1   3
   2   4

octave] b1=[-1; 1; 3]; b2=[2; -2; 3]; B=[b1 b2]
B =

  -1   2
   1  -2
   3   3

octave] C=B*A
C =

    3    5
   -3   -5
    9   21

octave] c1=B*a1; c2=B*a2; [c1 c2]
ans =

    3    5
   -3   -5
    9   21

octave]
```

CHAPTER 2

VECTOR SPACES

FORMAL RULES

1. Algebraic structures

1.1. Typical structures

A vector space has been introduced as a 4-tuple $\mathcal{V} = (V, S, +, \cdot)$ with specific behavior of the vector addition and scaling operations. Arithmetic operations between scalars were implicitly assumed to be similar to those of the real numbers, but also must be specified to obtain a complete definition of a vector space. Algebra defines various structures that specify the behavior operations with objects. Knowledge of these structures is useful not only in linear algebra, but also in other mathematical approaches to data analysis such as topology or geometry.

Groups. A group is a 2-tuple $\mathcal{G} = (G, +)$ containing a set G and an operation $+$ with properties from Table 2.2. If $\forall a, b \in G$, $a + b = b + a$, the group is said to be commutative. Besides the familiar example of integers under addition $(\mathbb{Z}, +)$, symmetry groups that specify spatial or functional relations are of particular interest. The rotations by $0, \frac{\pi}{2}, \pi, \frac{3\pi}{2}$ or vertices of a square form a group.

Addition rules	
$a + b \in G$	Closure
$a + (b + c) = (a + b) + c$	Associativity
$0 + a = a$	Identity element
$a + (-a) = 0$	Inverse element

Table 2.1. Group $\mathcal{G} = (G, +)$ properties, for $\forall a, b, c \in G$

Rings. A ring is a 3-tuple $\mathcal{R} = (R, +, \cdot)$ containing a set R and two operations $+, \cdot$ with properties from Table 2.1. As is often the case, a ring is more complex structure built up from simpler algebraic structures. With respect to addition a ring has the properties of a commutative group. Only associativity and existence of an identity element is imposed for multiplication. Matrix addition and multiplication has the structure of ring $(\mathbb{R}^{m \times m}, +, \cdot)$.

Addition rules	
$(R, +)$ is a commutative (Abelian) group	
Multiplication rules	
$a \cdot b \in R$	Closure
$(a \cdot b) \cdot c = a \cdot (b \cdot c)$	Associativity
$a \cdot 1 = 1 \cdot a = a$	Identity element
Distributivity	
$a \cdot (b + c) = (a \cdot b) + (a \cdot c)$	on the left
$(a + b) \cdot c = (a \cdot c) + (b \cdot c)$	on the right

Table 2.2. Ring $\mathcal{R} = (R, +, \cdot)$ properties, for $\forall a, b, c \in R$.

Fields. A ring is a 3-tuple $\mathcal{F} = (F, +, \cdot)$ containing a set F and two operations $+, \cdot$, each with properties of a commutative group, but with special behavior for the inverse of the null element. The multiplicative inverse is denoted as a^{-1}. Scalars S in the definition of a vector space must satisfy the properties of a field. Since the operations are often understood from context a field might be referred to as the full 3 – tuple, or, more concisely just through the set of elements as in the definition of a vector space.

Addition rules
$(F,+)$ is a commutative (Abelian) group
Multiplication rules
$(F,\cdot)$ is a commutative group except
that 0^{-1} does not exist
Distributivity
$a\cdot(b+c)=(a\cdot b)+(a\cdot c)$

Table 2.3. Field $\mathscr{R}=(F,+,\cdot)$ properties, for $\forall a,b,c\in F$.

Using the above definitions, a vector space $\mathcal{V}=(V,S,+,\cdot)$ can be described as a commutative group $(V,+)$ combined with a field S that satisfies the scaling properties $a\boldsymbol{u}\in V$, $a(\boldsymbol{u}+\boldsymbol{v})=a\boldsymbol{u}+b\boldsymbol{v}$, $(a+b)\,\boldsymbol{u}=a\boldsymbol{u}+b\boldsymbol{u}$, $a(b\boldsymbol{u})=(ab)\,\boldsymbol{u}$, $1\boldsymbol{u}=\boldsymbol{u}$, for $\forall a,b\in S$, $\forall \boldsymbol{u},\boldsymbol{v}\in V$.

1.2. Vector subspaces

A central interest in data science is to seek simple description of complex objects. A typical situation is that many instances of some object of interest are initially given as an m-tuple $\boldsymbol{v}\in\mathbb{R}^m$ with large m. Assuming that addition and scaling of such objects can cogently be defined, a vector space is obtained, say over the field of reals with an Euclidean distance, E_m. Examples include for instance recordings of medical data (electroencephalograms, electrocardiograms), sound recordings, or images, for which m can easily reach in to the millions. A natural question to ask is whether all the m real numbers are actually needed to describe the observed objects, or perhaps there is some intrinsic description that requires a much smaller number of descriptive parameters, that still preserves the useful idea of linear combination. The mathematical transcription of this idea is a vector subspace.

DEFINITION. (VECTOR SUBSPACE) . *$\mathcal{U}=(U,S,+,\cdot)$, $U\neq\emptyset$, is a vector subspace of vector space $\mathcal{V}=(V,S,+,\cdot)$ over the same field of scalars S, denoted by $\mathcal{U}\leq\mathcal{V}$, if $U\subseteq V$ and $\forall a,b\in S$, $\forall \boldsymbol{u},\boldsymbol{v}\in U$, the linear combination $a\boldsymbol{u}+b\boldsymbol{v}\in U$.*

The above states a vector subspace must be closed under linear combination, and have the same vector addition and scaling operations as the enclosing vector space. The simplest vector subspace of a vector space is the null subspace that only contains the null element, $U=\{\mathbf{0}\}$. In fact any subspace must contain the null element $\mathbf{0}$, or otherwise closure would not be verified for the particular linear combination $\boldsymbol{u}+(-\boldsymbol{u})=\mathbf{0}$. If $U\subset V$, then $\mathcal{U}$ is said to be a *proper subspace* of $\mathcal{V}$, denoted by $\mathcal{U}<\mathcal{V}$.

Setting $n-m$ components equal to zero in the real space $\mathscr{R}_m$ defines a proper subspace whose elements can be placed into a one-to-one correspondence with the vectors within $\mathscr{R}_n$. For example, setting component m of $\boldsymbol{x}\in\mathbb{R}^m$ equal to zero gives $\boldsymbol{x}=[\ x_1\ x_2\ \ldots\ x_{m-1}\ 0\ ]^T$ that while not a member of $\mathbb{R}^{m-1}$, is in a one-to-one relation with $\boldsymbol{x}'=[\ x_1\ x_2\ \ldots\ x_{m-1}\ ]^T\in\mathbb{R}^{m-1}$. Dropping the last component of $\boldsymbol{y}\in\mathbb{R}^m$, $\boldsymbol{y}=[\ y_1\ y_2\ \ldots\ y_{m-1}\ y_m\ ]^T$ gives vector $\boldsymbol{y}'=[\ y_1\ y_2\ \ldots\ y_{m-1}\ ]\in\mathbb{R}^{m-1}$, but this is no longer a one-to-one correspondence since for some given $\boldsymbol{y}'$, the last component y_m could take any value.

```
octave] m=3; x=[1; 2; 0]; xp=x(1:2); disp(xp)
```

```
   1
   2
```

```
octave] y=[1; 2; 3]; yp=y(1:2); disp(yp)
   1
   2
octave]
```

Vector subspaces arise in decomposition of a vector space. The converse, composition of vector spaces $\mathcal{U}=(U,S,+,\cdot)$ $\mathcal{V}=(V,S,+,\cdot)$ is also defined in terms of linear combination. A vector $\boldsymbol{x}\in\mathbb{R}^3$ can be obtained as the linear combination

$$\boldsymbol{x}=\begin{bmatrix}x_1\\x_2\\x_3\end{bmatrix}=\begin{bmatrix}x_1\\0\\0\end{bmatrix}+\begin{bmatrix}0\\x_2\\x_3\end{bmatrix},$$

but also as

$$\boldsymbol{x}=\begin{bmatrix}x_1\\x_2\\x_3\end{bmatrix}=\begin{bmatrix}x_1\\x_2-a\\0\end{bmatrix}+\begin{bmatrix}0\\a\\x_3\end{bmatrix},$$

for some arbitrary $a\in\mathbb{R}$. In the first case, $\boldsymbol{x}$ is obtained as a unique linear combination of a vector from the set $U=\{\begin{bmatrix}x_1&0&0\end{bmatrix}^T \mid x_1\in\mathbb{R}\}$ with a vector from $V=\{\begin{bmatrix}0&x_2&x_3\end{bmatrix}^T \mid x_2,x_3\in\mathbb{R}\}$. In the second case, there is an infinity of linear combinations of a vector from V with another from $W=\{\begin{bmatrix}x_1&x_2&0\end{bmatrix}^T \mid x_1,x_2\in\mathbb{R}\}$ to the vector $\boldsymbol{x}$. This is captured by a pair of definitions to describe vector space composition.

DEFINITION. *Given two vector subspaces $\mathcal{U}=(U,S,+,\cdot)$, $\mathcal{V}=(V,S,+,\cdot)$ of the space $\mathcal{W}=(W,S,+,\cdot)$, the sum is the vector space $\mathcal{U}+\mathcal{V}=(U+V,S,+,\cdot)$, where the sum of the two sets of vectors U,V is $U+V=\{\boldsymbol{u}+\boldsymbol{v} \mid \boldsymbol{u}\in U,\boldsymbol{v}\in V\}$.*

DEFINITION. *Given two vector subspaces $\mathcal{U}=(U,S,+,\cdot)$, $\mathcal{V}=(V,S,+,\cdot)$ of the space $\mathcal{W}=(W,S,+,\cdot)$, the direct sum is the vector space $\mathcal{U}\oplus\mathcal{V}=(U\oplus V,S,+,\cdot)$, where the direct sum of the two sets of vectors U,V is $U\oplus V=\{\boldsymbol{u}+\boldsymbol{v} \mid \exists!\,\boldsymbol{u}\in U,\exists!\,\boldsymbol{v}\in V\}$. (unique decomposition)*

Since the same scalar field, vector addition, and scaling is used , it is more convenient to refer to vector space sums simply by the sum of the vector sets $U+V$, or $U\oplus V$, instead of specifying the full tuplet for each space. This shall be adopted henceforth to simplify the notation.

```
octave] u=[1; 0; 0]; v=[0; 2; 3]; vp=[0; 1; 3]; w=[1; 1; 0]; disp([u+v vp+w])
   1   1
   2   2
   3   3
octave]
```

In the previous example, the essential difference between the two ways to express $\boldsymbol{x} \in \mathbb{R}^3$ is that $U \cap V = \{\mathbf{0}\}$, but $V \cap W = \{[\ 0\ \ a\ \ 0\ ]^T \mid a \in \mathbb{R}\} \neq \{\mathbf{0}\}$, and in general if the zero vector is the only common element of two vector spaces then the sum of the vector spaces becomes a direct sum. In practice, the most important procedure to construct direct sums or check when an intersection of two vector subspaces reduces to the zero vector is through an inner product.

DEFINITION. *Two vector subspaces U, V of the real vector space $\mathbb{R}^m$ are orthogonal, denoted as $U \perp V$ if $\boldsymbol{u}^T\boldsymbol{v} = 0$ for any $\boldsymbol{u} \in U, \boldsymbol{v} \in V$.*

DEFINITION. *Two vector subspaces U,V of $U + V$ are orthogonal complements, denoted $U = V^\perp$, $V = U^\perp$ if they are orthogonal subspaces, $U \perp V$, and $U \cap V = \{\mathbf{0}\}$, i.e., the null vector is the only common element of both subspaces.*

```
octave] disp([u'*v vp'*w])
   0   1
octave]
```

The above concept of orthogonality can be extended to other vector subspaces, such as spaces of functions. It can also be extended to other choices of an inner product, in which case the term conjugate vector spaces is sometimes used.

The concepts of sum and direct sum of vector spaces used linear combinations of the form $\boldsymbol{u} + \boldsymbol{v}$. This notion can be extended to arbitrary linear combinations.

DEFINITION. *In vector space $\mathcal{U} = (V, S, +, \cdot)$, the span of vectors $\boldsymbol{a}_1, \boldsymbol{a}_2, \ldots, \boldsymbol{a}_n \in V$, is the set of vectors reachable by linear combination*

$$\text{span}\{\boldsymbol{a}_1, \boldsymbol{a}_2, \ldots, \boldsymbol{a}_n\} = \{\boldsymbol{b} \in V \mid \exists x_1, \ldots, x_n \in S \text{ such that } \boldsymbol{b} = x_1\boldsymbol{a}_1 + \ldots + x_n\boldsymbol{a}_n\}.$$

Note that for real vector spaces a member of the span of the vectors $\{\boldsymbol{a}_1, \boldsymbol{a}_2, \ldots, \boldsymbol{a}_n\}$ is the vector $\boldsymbol{b}$ obtained from the matrix vector multiplication

$$\boldsymbol{b} = \boldsymbol{A}\boldsymbol{x} = \begin{bmatrix} \boldsymbol{a}_1 & \boldsymbol{a}_2 & \ldots & \boldsymbol{a}_n \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}.$$

From the above, the span is a subset of the co-domain of the linear mapping $\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x}$.

2. Vector subspaces of a linear mapping

The wide-ranging utility of linear algebra essentially results a complete characterization of the behavior of a linear mapping between vector spaces $\boldsymbol{f}: U \longrightarrow V$, $\boldsymbol{f}(a\boldsymbol{u} + b\boldsymbol{v}) = a\boldsymbol{f}(\boldsymbol{u}) + b\boldsymbol{f}(\boldsymbol{v})$. For some given linear mapping the questions that arise are:

1. Can any vector within V be obtained by evaluation of $\boldsymbol{f}$?

2. Is there a single way that a vector within V can be obtained by evaluation of $\boldsymbol{f}$?

Linear mappings between real vector spaces $\boldsymbol{f}: \mathbb{R}^n \longrightarrow \mathbb{R}^m$, have been seen to be completely specified by a matrix $\boldsymbol{A} \in \mathbb{R}^{m \times n}$. It is common to frame the above questions about the behavior of the linear mapping $\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x}$ through sets associated with the matrix $\boldsymbol{A}$. To frame an answer to the first question, a set of reachable vectors is first defined.

DEFINITION. *The column space (or range) of matrix $\boldsymbol{A} \in \mathbb{R}^{m \times n}$ is the set of vectors reachable by linear combination of the matrix column vectors*

$$C(\boldsymbol{A}) = \text{range}(\boldsymbol{A}) = \{\boldsymbol{b} \in \mathbb{R}^m \mid \exists \boldsymbol{x} \in \mathbb{R}^n \text{such that } \boldsymbol{b} = \boldsymbol{A}\boldsymbol{x}\}.$$

By definition, the column space is included in the co-domain of the function $\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x}$, $C(\boldsymbol{A}) \subseteq \mathbb{R}^m$, and is readily seen to be a vector subspace of $\mathbb{R}^m$. The question that arises is whether the column space is the entire co-domain $C(\boldsymbol{A}) = \mathbb{R}^m$ that would signify that any vector can be reached by linear combination. If this is not the case then the column space would be a proper subset, $C(\boldsymbol{A}) \subset \mathbb{R}^m$, and the question is to determine what part of the co-domain cannot be reached by linear combination of columns of $\boldsymbol{A}$. Consider the orthogonal complement of $C(\boldsymbol{A})$ defined as the set vectors orthogonal to all of the column vectors of $\boldsymbol{A}$, expressed through inner products as

$$\boldsymbol{a}_1^T \boldsymbol{y} = 0, \boldsymbol{a}_2^T \boldsymbol{y} = 0, \ldots, \boldsymbol{a}_n^T \boldsymbol{y} = 0.$$

This can be expressed more concisely through the transpose operation

$$\boldsymbol{A} = \begin{bmatrix} \boldsymbol{a}_1 & \boldsymbol{a}_2 & \ldots & \boldsymbol{a}_n \end{bmatrix}, \boldsymbol{A}^T \boldsymbol{y} = \begin{bmatrix} \boldsymbol{a}_1^T \\ \boldsymbol{a}_2^T \\ \vdots \\ \boldsymbol{a}_n^T \end{bmatrix} = \begin{bmatrix} \boldsymbol{a}_1^T \boldsymbol{y} \\ \boldsymbol{a}_2^T \boldsymbol{y} \\ \vdots \\ \boldsymbol{a}_n^T \boldsymbol{y} \end{bmatrix},$$

and leads to the definition of a set of vectors for which $\boldsymbol{A}^T \boldsymbol{y} = \boldsymbol{0}$

DEFINITION. *The left null space (or cokernel) of a matrix $\boldsymbol{A} \in \mathbb{R}^{m \times n}$ is the set*

$$N(\boldsymbol{A}^T) = \text{null}(\boldsymbol{A}^T) = \{\boldsymbol{y} \in \mathbb{R}^m \mid \boldsymbol{A}^T \boldsymbol{y} = \boldsymbol{0}\}.$$

Note that the left null space is also a vector subspace of the co-domain of $\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x}$, $N(\boldsymbol{A}^T) \subseteq \mathbb{R}^m$. The above definitions suggest that both the matrix and its transpose play a role in characterizing the behavior of the linear mapping $\boldsymbol{f} = \boldsymbol{A}\boldsymbol{x}$, so analagous sets are define for the transpose $\boldsymbol{A}^T$.

DEFINITION. *The row space (or corange) of a matrix $\boldsymbol{A} \in \mathbb{R}^{m \times n}$ is the set*

$$R(\boldsymbol{A}) = C(\boldsymbol{A}^T) = \text{range}(\boldsymbol{A}^T) = \{\boldsymbol{c} \in \mathbb{R}^n \mid \exists \boldsymbol{y} \in \mathbb{R}^m \, \boldsymbol{c} = \boldsymbol{A}^T \boldsymbol{y}\} \subseteq \mathbb{R}^n$$

DEFINITION. *The null space of a matrix $\boldsymbol{A} \in \mathbb{R}^{m\times n}$ is the set*

$$N(\boldsymbol{A}) = \text{null}(\boldsymbol{A}) = \{\boldsymbol{x} \in \mathbb{R}^n \mid \boldsymbol{A}\boldsymbol{x} = \boldsymbol{0}\} \subseteq \mathbb{R}^n$$

Examples. Consider a linear mapping between real spaces $\boldsymbol{f}: \mathbb{R}^n \longrightarrow \mathbb{R}^m$, defined by $\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x} = [\ y_1\ \ \ldots\ \ y_n\ ]^T$, with $\boldsymbol{A} \in \mathbb{R}^{m\times n}$.

1. For $n = 1$, $m = 3$,

$$\boldsymbol{A} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \boldsymbol{A}^T = [\ 1\ \ 0\ \ 0\ ],$$

the column space $C(\boldsymbol{A})$ is the y_1-axis, and the left null space $N(\boldsymbol{A}^T)$ is the y_2y_3-plane. Vectors that span these spaces are returned by the Octave `orth` and `null` functions.

```
octave] A=[1; 0; 0]; disp(orth(A));
        disp('-----');
        disp(null(A'))
   -1
   -0
   -0
 -----
    0    0
    1    0
    0    1
octave]
```

2. For $n = 2$, $m = 3$,

$$\boldsymbol{A} = \begin{bmatrix} 1 & -1 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} = [\ \boldsymbol{a}_1\ \ \boldsymbol{a}_2\ ], \boldsymbol{A}^T = \begin{bmatrix} 1 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix},$$

the columns of $\boldsymbol{A}$ are colinear, $\boldsymbol{a}_2 = -\boldsymbol{a}_1$, and the column space $C(\boldsymbol{A})$ is the y_1-axis, and the left null space $N(\boldsymbol{A}^T)$ is the y_2y_3-plane, as before.

```
octave] A=[1 -1; 0 0; 0 0];
        disp(orth(A));
        disp('-----');
        disp(null(A'))
   -1.00000
   -0.00000
   -0.00000
 -----
    0    0
    1    0
    0    1
octave]
```

3. For $n = 2$, $m = 3$,

$$\boldsymbol{A} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix}, \boldsymbol{A}^T = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix},$$

the column space $C(\boldsymbol{A})$ is the y_1y_2-plane, and the left null space $N(\boldsymbol{A}^T)$ is the y_3-axis.

```
octave] A=[1 0; 0 1; 0 0];
        disp(orth(A));
        disp('-----');
        disp(null(A'))
   -1   -0
   -0   -1
   -0   -0
 -----
    0
    0
    1
octave]
```

4. For $n = 2$, $m = 3$,

$$\boldsymbol{A} = \begin{bmatrix} 1 & 1 \\ 1 & -1 \\ 0 & 0 \end{bmatrix}, \boldsymbol{A}^T = \begin{bmatrix} 1 & 1 & 0 \\ 1 & -1 & 0 \end{bmatrix},$$

the same $C(\boldsymbol{A})$, $N(\boldsymbol{A}^T)$ are obtained, albeit with a different set of spanning vectors returned by `orth`.

```
octave] A=[1 1; 1 -1; 0 0];
        disp(orth(A));
        disp('-----');
        disp(null(A'))
    0.70711    0.70711
    0.70711   -0.70711
   -0.00000   -0.00000
 -----
    0
    0
    1
octave]
```

5. For $n=3$, $m=3$,

$$\boldsymbol{A}=\begin{bmatrix}1&1&3\\1&-1&-1\\1&1&3\end{bmatrix}=\begin{bmatrix}\boldsymbol{a}_1&\boldsymbol{a}_2&\boldsymbol{a}_3\end{bmatrix},$$

$$\boldsymbol{A}^T=\begin{bmatrix}1&1&1\\1&-1&1\\3&-1&3\end{bmatrix}=\begin{bmatrix}\boldsymbol{a}_1^T\\\boldsymbol{a}_2^T\\\boldsymbol{a}_3^T\end{bmatrix},\boldsymbol{A}^T\boldsymbol{y}=\begin{bmatrix}\boldsymbol{a}_1^T\boldsymbol{y}\\\boldsymbol{a}_2^T\boldsymbol{y}\\\boldsymbol{a}_3^T\boldsymbol{y}\end{bmatrix}$$

since $\boldsymbol{a}_3=\boldsymbol{a}_1+2\boldsymbol{a}_2$, the orthogonality condition $\boldsymbol{A}^T\boldsymbol{y}=\boldsymbol{0}$ is satisfied by vectors of form $\boldsymbol{y}=\begin{bmatrix}a&0&-a\end{bmatrix}$, $a\in\mathbb{R}$.

```
octave] A=[1 1 3; 1 -1 -1; 1 1 3];
        disp(orth(A));
        disp('-----');
        disp(null(A'))
   0.69157   0.14741
  -0.20847   0.97803
   0.69157   0.14741
 -----
   0.70711
   0.00000
  -0.70711
octave]
```

The above low dimensional examples are useful to gain initial insight into the significance of the spaces $C(\boldsymbol{A}), N(\boldsymbol{A}^T)$. Further appreciation can be gained by applying the same concepts to processing of images. A gray-scale image of size p_x by p_y pixels can be represented as a vector with $m=p_xp_y$ components, $\boldsymbol{b}\in[0,1]^m\subset\mathbb{R}^m$. Even for a small image with $p_x=p_y=128=2^7$ pixels along each direction, the vector $\boldsymbol{b}$ would have $m=2^{14}$ components. An image can be specified as a linear combination of the columns of the identity matrix

$$\boldsymbol{b}=\boldsymbol{I}\boldsymbol{b}=\begin{bmatrix}\boldsymbol{e}_1&\boldsymbol{e}_2&\dots&\boldsymbol{e}_m\end{bmatrix}\begin{bmatrix}b_1\\b_2\\\vdots\\b_m\end{bmatrix},$$

with b_i the gray-level intensity in pixel i. Similar to the inclined plane example from §1, an alternative description as a linear combination of another set of vectors $\boldsymbol{a}_1,\dots,\boldsymbol{a}_m$ might be more relevant. One choice of greater utility for image processing mimics the behavior of the set $\{1,\cos t,\cos 2t,\dots,\sin t,\sin 2t,\dots\}$ that extends the second example in §1, would be for $m=4$

$$\boldsymbol{A}=\begin{bmatrix}\boldsymbol{a}_1&\boldsymbol{a}_2&\boldsymbol{a}_3&\boldsymbol{a}_4\end{bmatrix}=\begin{bmatrix}1&1&1&0\\1&1&0&1\\1&0&1&1\\1&0&0&0\end{bmatrix}.$$

DATA REDUNDANCY

1. Linear dependence

For the simple scalar mapping $f:\mathbb{R}\longrightarrow\mathbb{R}$, $f(x)=ax$, the condition $f(x)=0$ implies either that $a=0$ or $x=0$. Note that $a=0$ can be understood as defining a zero mapping $f(x)=0$. Linear mappings between vector spaces, $\boldsymbol{f}:U\longrightarrow V$, can exhibit different behavior, and the condtion $\boldsymbol{f}(\boldsymbol{x})=\boldsymbol{A}\boldsymbol{x}=\boldsymbol{0}$, might be satisfied for both $\boldsymbol{x}\neq\boldsymbol{0}$, and $\boldsymbol{A}\neq\boldsymbol{0}$. Analogous to the scalar case, $\boldsymbol{A}=\boldsymbol{0}$ can be understood as defining a zero mapping, $\boldsymbol{f}(\boldsymbol{x})=\boldsymbol{0}$.

In vector space $\mathcal{U}=(V,S,+,\cdot)$, vectors $\boldsymbol{u},\boldsymbol{v}\in V$ related by a scaling operation, $\boldsymbol{v}=a\boldsymbol{u}$, $a\in S$, are said to be colinear, and are considered to contain redundant data. This can be restated as $\boldsymbol{v}\in\text{span}\{\boldsymbol{u}\}$, from which it results that $\text{span}\{\boldsymbol{u}\}=\text{span}\{\boldsymbol{u},\boldsymbol{v}\}$. Colinearity can be expressed only in terms of vector scaling, but other types of redundancy arise when also considering vector addition as expressed by the span of a vector set. Assuming that $\boldsymbol{v}\notin\text{span}\{\boldsymbol{u}\}$, then the strict inclusion relation $\text{span}\{\boldsymbol{u}\}\subset\text{span}\{\boldsymbol{u},\boldsymbol{v}\}$ holds. This strict inclusion expressed in terms of set concepts can be transcribed into an algebraic condition.

DEFINITION. *The vectors $\boldsymbol{a}_1, \boldsymbol{a}_2, \ldots, \boldsymbol{a}_n \in V$, are linearly dependent if there exist n scalars, $x_1, \ldots, x_n \in S$, at least one of which is different from zero such that*

$$x_1 \boldsymbol{a}_1 + \ldots + x_n \boldsymbol{a}_n = \boldsymbol{0}.$$

Introducing a matrix representation of the vectors

$$\boldsymbol{A} = \begin{bmatrix} \boldsymbol{a}_1 & \boldsymbol{a}_2 & \ldots & \boldsymbol{a}_n \end{bmatrix}; \boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

allows restating linear dependence as the existence of a non-zero vector, $\exists \boldsymbol{x} \neq \boldsymbol{0}$, such that $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{0}$. Linear dependence can also be written as $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{0} \nRightarrow \boldsymbol{x} = \boldsymbol{0}$, or that one cannot deduce from the fact that the linear mapping $\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x}$ attains a zero value that the argument itself is zero. The converse of this statement would be that the only way to ensure $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{0}$ is for $\boldsymbol{x} = \boldsymbol{0}$, or $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{0} \Longrightarrow \boldsymbol{x} = \boldsymbol{0}$, leading to the concept of linear independence.

DEFINITION. *The vectors $\boldsymbol{a}_1, \boldsymbol{a}_2, \ldots, \boldsymbol{a}_n \in V$, are linearly independent if the only n scalars, $x_1, \ldots, x_n \in S$, that satisfy*

$$x_1 \boldsymbol{a}_1 + \ldots + x_n \boldsymbol{a}_n = \boldsymbol{0}, \tag{2.1}$$

are $x_1 = 0$, $x_2 = 0$,...,$x_n = 0$.

2. Basis and dimension

Vector spaces are closed under linear combination, and the span of a vector set $\mathscr{B} = \{\boldsymbol{a}_1, \boldsymbol{a}_2, \ldots\}$ defines a vector subspace. If the entire set of vectors can be obtained by a spanning set, $V = \operatorname{span} \mathscr{B}$, extending $\mathscr{B}$ by an additional element $\mathbb{C} = \mathscr{B} \cup \{\boldsymbol{b}\}$ would be redundant since $\operatorname{span} \mathscr{B} = \operatorname{span} \mathbb{C}$. This is recognized by the concept of a basis, and also allows leads to a characterization of the size of a vector space by the cardinality of a basis set.

DEFINITION. *A set of vectors $\boldsymbol{u}_1, \ldots, \boldsymbol{u}_n \in V$ is a basis for vector space $\mathcal{U} = (V, S, +, \cdot)$ if*

1. *$\boldsymbol{u}_1, \ldots, \boldsymbol{u}_n$ are linearly independent;*
2. *$\operatorname{span}\{\boldsymbol{u}_1, \ldots, \boldsymbol{u}_n\} = V$.*

DEFINITION. *The number of vectors $\boldsymbol{u}_1, \ldots, \boldsymbol{u}_n \in V$ within a basis is the dimension of the vector space $\mathcal{U} = (V, S, +, \cdot)$.*

3. Dimension of matrix spaces

The domain and co-domain of the linear mapping $\boldsymbol{f}: U \longrightarrow V$, $\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x}$, are decomposed by the spaces associated with the matrix $\boldsymbol{A}$. When $U = \mathbb{R}^n$, $V = \mathbb{R}^m$, the following vector subspaces associated with the matrix $\boldsymbol{A} \in \mathbb{R}^{m \times n}$ have been defined:

- $C(\boldsymbol{A})$ the column space of $\boldsymbol{A}$
- $C(\boldsymbol{A}^T)$ the row space of $\boldsymbol{A}$
- $N(\boldsymbol{A})$ the null space of $\boldsymbol{A}$
- $N(\boldsymbol{A}^T)$ the left null space of $\boldsymbol{A}$, or null space of $\boldsymbol{A}^T$

DEFINITION. *The rank of a matrix $\boldsymbol{A} \in \mathbb{R}^{m \times n}$ is the dimension of its column space and is equal to the dimension of its row space.*

DEFINITION. *The nullity of a matrix $\boldsymbol{A} \in \mathbb{R}^{m \times n}$ is the dimension of its null space.*

CHAPTER 3
FUNDAMENTAL THEOREM OF LINEAR ALGEBRA

DATA INFORMATION

1. Partition of linear mapping domain and codomain

A partition of a set S has been introduced as a collection of subsets $P=\{S_i \mid S_i \subset P, S_i \neq \emptyset\}$ such that any given element $x \in S$ belongs to only one set in the partition. This is modified when applied to subspaces of a vector space, and a partition of a set of vectors is understood as a collection of subsets such that any vector except $\mathbf{0}$ belongs to only one member of the partition.

Linear mappings between vector spaces $\boldsymbol{f}: U \longrightarrow V$ can be represented by matrices $\boldsymbol{A}$ with columns that are images of the columns of a basis $\{\boldsymbol{u}_1, \boldsymbol{u}_2, \dots\}$ of U

$$\boldsymbol{A} = \begin{bmatrix} \boldsymbol{f}(\boldsymbol{u}_1) & \boldsymbol{f}(\boldsymbol{u}_2) & \dots \end{bmatrix}.$$

Consider the case of real finite-dimensional domain and co-domain, $\boldsymbol{f}: \mathbb{R}^n \longrightarrow \mathbb{R}^m$, in which case $\boldsymbol{A} \in \mathbb{R}^{m \times n}$,

$$\boldsymbol{A} = \begin{bmatrix} \boldsymbol{f}(\boldsymbol{e}_1) & \boldsymbol{f}(\boldsymbol{e}_2) & \dots & \boldsymbol{f}(\boldsymbol{e}_n) \end{bmatrix} = \begin{bmatrix} \boldsymbol{a}_1 & \boldsymbol{a}_2 & \dots & \boldsymbol{a}_n \end{bmatrix}.$$

The column space of $\boldsymbol{A}$ is a vector subspace of the codomain, $C(\boldsymbol{A}) \leq \mathbb{R}^m$, but according to the definition of dimension if $n < m$ there remain non-zero vectors within the codomain that are outside the range of $\boldsymbol{A}$,

$$n < m \Longrightarrow \exists \boldsymbol{v} \in \mathbb{R}^m, \boldsymbol{v} \neq \mathbf{0}, \boldsymbol{v} \notin C(\boldsymbol{A}).$$

All of the non-zero vectors in $N(\boldsymbol{A}^T)$, namely the set of vectors orthogonal to all columns in $\boldsymbol{A}$ fall into this category. The above considerations can be stated as

$$C(\boldsymbol{A}) \leq \mathbb{R}^m, \;\; N(\boldsymbol{A}^T) \leq \mathbb{R}^m, \;\; C(\boldsymbol{A}) \perp N(\boldsymbol{A}^T) \;\; C(\boldsymbol{A}) + N(\boldsymbol{A}^T) \leq \mathbb{R}^m \, .$$

The question that arises is whether there remain any non-zero vectors in the codomain that are not part of $C(\boldsymbol{A})$ or $N(\boldsymbol{A}^T)$. The fundamental theorem of linear algebra states that there no such vectors, that $C(\boldsymbol{A})$ is the orthogonal complement of $N(\boldsymbol{A}^T)$, and their direct sum covers the entire codomain $C(\boldsymbol{A}) \oplus N(\boldsymbol{A}^T) = \mathbb{R}^m$.

LEMMA 3.1. *Let $\mathcal{U}, \mathcal{V}$, be subspaces of vector space $\mathcal{W}$. Then $\mathcal{W} = \mathcal{U} \oplus \mathcal{V}$ if and only if*

i. $\mathcal{W} = \mathcal{U} + \mathcal{V}$, and

ii. $\mathcal{U} \cap \mathcal{V} = \{\mathbf{0}\}$.

Proof. *$\mathcal{W} = \mathcal{U} \oplus \mathcal{V} \Longrightarrow \mathcal{W} = \mathcal{U} + \mathcal{V}$ by definition of direct sum, sum of vector subspaces. To prove that $\mathcal{W} = \mathcal{U} \oplus \mathcal{V} \Longrightarrow \mathcal{U} \cap \mathcal{V} = \{\mathbf{0}\}$, consider $\boldsymbol{w} \in \mathcal{U} \cap \mathcal{V}$. Since $\boldsymbol{w} \in \mathcal{U}$ and $\boldsymbol{w} \in \mathcal{V}$ write*

$$\boldsymbol{w} = \boldsymbol{w} + \mathbf{0} \;\; (\boldsymbol{w} \in \mathcal{U}, \mathbf{0} \in \mathcal{V}), \;\; \boldsymbol{w} = \mathbf{0} + \boldsymbol{w} \;\; (\mathbf{0} \in \mathcal{U}, \boldsymbol{w} \in \mathcal{V}),$$

and since expression $\boldsymbol{w} = \boldsymbol{u} + \boldsymbol{v}$ is unique, it results that $\boldsymbol{w} = \mathbf{0}$. Now assume (i),(ii) and establish an unique decomposition. Assume there might be two decompositions of $\boldsymbol{w} \in \mathcal{W}$, $\boldsymbol{w} = \boldsymbol{u}_1 + \boldsymbol{v}_1$, $\boldsymbol{w} = \boldsymbol{u}_2 + \boldsymbol{v}_2$, with $\boldsymbol{u}_1, \boldsymbol{u}_2 \in \mathcal{U}$, $\boldsymbol{v}_1, \boldsymbol{v}_2 \in \mathcal{V}$. Obtain $\boldsymbol{u}_1 + \boldsymbol{v}_1 = \boldsymbol{u}_2 + \boldsymbol{v}_2$, or $\boldsymbol{x} = \boldsymbol{u}_1 - \boldsymbol{u}_2 = \boldsymbol{v}_2 - \boldsymbol{v}_1$. Since $\boldsymbol{x} \in \mathcal{U}$ and $\boldsymbol{x} \in \mathcal{V}$ it results that $\boldsymbol{x} = \mathbf{0}$, and $\boldsymbol{u}_1 = \boldsymbol{u}_2$, $\boldsymbol{v}_1 = \boldsymbol{v}_2$, i.e., the decomposition is unique. □

In the vector space $U + V$ the subspaces U, V are said to be orthogonal complements is $U \perp V$, and $U \cap V = \{\mathbf{0}\}$. When $U \leq \mathbb{R}^m$, the orthogonal complement of U is denoted as $U^\perp$, $U \oplus U^\perp = \mathbb{R}^m$.

THEOREM. *Given the linear mapping associated with matrix $\boldsymbol{A} \in \mathbb{R}^{m \times n}$ we have:*

1. *$C(\boldsymbol{A}) \oplus N(\boldsymbol{A}^T) = \mathbb{R}^m$, the direct sum of the column space and left null space is the codomain of the mapping*
2. *$C(\boldsymbol{A}^T) \oplus N(\boldsymbol{A}) = \mathbb{R}^n$, the direct sum of the row space and null space is the domain of the mapping*
3. *$C(\boldsymbol{A}) \perp N(\boldsymbol{A}^T)$ and $C(\boldsymbol{A}) \cap N(\boldsymbol{A}^T) = \{\mathbf{0}\}$, the column space is orthogonal to the left null space, and they are orthogonal complements of one another,*

$$C(\boldsymbol{A}) = N(\boldsymbol{A}^T)^\perp, \;\; N(\boldsymbol{A}^T) = C(\boldsymbol{A})^\perp \, .$$

4. *$C(A^T)\perp N(A)$ and $C(A^T)\cap N(A)=\{0\}$, the row space is orthogonal to the null space, and they are orthogonal complements of one another,*

$$C(A^T)=N(A)^\perp,\ \ N(A)=C(A^T)^\perp\,.$$

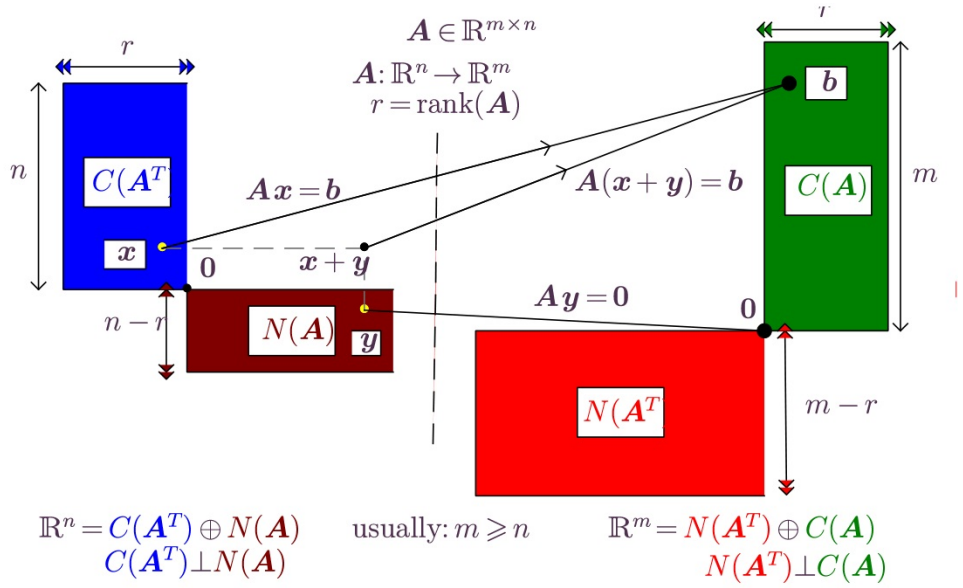


Figure 3.1. Graphical represenation of the Fundamental Theorem of Linear Algebra, Gil Strang, *Amer. Math. Monthly* **100**, 848-855, 1993.

Consideration of equality between sets arises in proving the above theorem. A standard technique to show set equality $A=B$, is by double inclusion, $A\subseteq B\wedge B\subseteq A\Longrightarrow A=B$. This is shown for the statements giving the decomposition of the codomain $\mathbb{R}^m$. A similar approach can be used to decomposition of $\mathbb{R}^n$.

i. $C(A)\perp N(A^T)$ (column space is orthogonal to left null space).

Proof. Consider arbitrary $u\in C(A), v\in N(A^T)$. By definition of $C(A)$, $\exists x\in\mathbb{R}^n$ such that $u=Ax$, and by definition of $N(A^T)$, $A^Tv=0$. Compute $u^Tv=(Ax)^Tv=x^TA^Tv=x^T(A^Tv)=x^T0=0$, hence $u\perp v$ for arbitrary u,v, and $C(A)\perp N(A^T)$. □

ii. $C(A)\cap N(A^T)=\{0\}$ (0 is the only vector both in $C(A)$ and $N(A^T)$).

Proof. (By contradiction, *reductio ad absurdum*). Assume there might be $b\in C(A)$ and $b\in N(A^T)$ and $b\neq 0$. Since $b\in C(A)$, $\exists x\in\mathbb{R}^n$ such that $b=Ax$. Since $b\in N(A^T)$, $A^Tb=A^T(Ax)=0$. Note that $x\neq 0$ since $x=0\Longrightarrow b=0$, contradicting assumptions. Multiply equality $A^TAx=0$ on left by x^T,

$$x^TA^TAx=0\Longrightarrow(Ax)^T(Ax)=b^Tb=\|b\|^2=0,$$

thereby obtaining $b=0$, using norm property 3. Contradiction.

□

iii. $C(A)\oplus N(A^T)=\mathbb{R}^m$

Proof. (iii) and (iv) have established that $C(A), N(A^T)$ are orthogonal complements

$$C(A)=N(A^T)^\perp, N(A^T)=C(A)^\perp.$$

By Lemma 2 it results that $C(\boldsymbol{A}) \oplus N(\boldsymbol{A}^T) = \mathbb{R}^m$. □

The remainder of the FTLA is established by considering $\boldsymbol{B} = \boldsymbol{A}^T$, e.g., since it has been established in (v) that $C(\boldsymbol{B}) \oplus N(\boldsymbol{A}^T) = \mathbb{R}^n$, replacing $\boldsymbol{B} = \boldsymbol{A}^T$ yields $C(\boldsymbol{A}^T) \oplus N(\boldsymbol{A}) = \mathbb{R}^m$, etc.

DATA PARTITIONING

1. Mappings as data

1.1. Vector spaces of mappings and matrix representations

A vector space $\mathscr{L}$ can be formed from all linear mappings from the vector space $\mathcal{U} = (U, S, +, \cdot)$ to another vector space $\mathcal{V} = (V, S, +, \cdot)$

$$\mathscr{L} = \{L, S, +, \cdot\}, \quad L = \{\boldsymbol{f} \mid \boldsymbol{f} : U \longrightarrow V, \boldsymbol{f}(a\boldsymbol{u} + b\boldsymbol{v}) = a\boldsymbol{f}(\boldsymbol{u}) + b\boldsymbol{f}(\boldsymbol{v})\},$$

with addition and scaling of linear mappings defined by $(\boldsymbol{f} + \boldsymbol{g})(\boldsymbol{u}) = \boldsymbol{f}(\boldsymbol{u}) + \boldsymbol{g}(\boldsymbol{u})$ and $(a\boldsymbol{f})(\boldsymbol{u}) = a\boldsymbol{f}(\boldsymbol{u})$. Let $B = \{\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots\}$ denote a basis for the domain U of linear mappings within $\mathscr{L}$, such that the linear mapping $\boldsymbol{f} \in \mathscr{L}$ is represented by the matrix

$$\boldsymbol{A} = \begin{bmatrix} \boldsymbol{f}(\boldsymbol{u}_1) & \boldsymbol{f}(\boldsymbol{u}_2) & \ldots \end{bmatrix}.$$

When the domain and codomain are the real vector spaces $U = \mathbb{R}^n$, $V = \mathbb{R}^m$, the above is a standard matrix of real numbers, $\boldsymbol{A} \in \mathbb{R}^{m \times n}$. For linear mappings between infinite dimensional vector spaces the matrix is understood in a generalized sense to contain an infinite number of columns that are elements of the codomain V. For example, the indefinite integral is a linear mapping between the vector space of functions that allow differentiation to any order,

$$\int : C^\infty \longrightarrow C^\infty \quad v(x) = \int u(x)\,\mathrm{d}x$$

and for the monomial basis $B = \{1, x, x^2, \ldots\}$, is represented by the generalized matrix

$$\boldsymbol{A} = \begin{bmatrix} x & \frac{1}{2}x^2 & \frac{1}{3}x^3 & \ldots \end{bmatrix}.$$

Truncation of the basis expansion $u(x) = \sum_{j=1}^{\infty} u_j x^j$ where $u_j \in \mathbb{R}$ to n terms, and sampling of $u \in C^\infty$ at points $x_1, \ldots, x_m$, forms a standard matrix of real numbers

$$\boldsymbol{A} = \begin{bmatrix} \boldsymbol{x} & \frac{1}{2}\boldsymbol{x}^2 & \frac{1}{3}\boldsymbol{x}^3 & \ldots \end{bmatrix} \in \mathbb{R}^{m \times n}, \quad \boldsymbol{x}^j = \begin{bmatrix} x_1^j \\ \vdots \\ x_m^j \end{bmatrix}.$$

As to be expected, matrices can also be organized as vector space $\mathscr{M}$, which is essentially the representation of the associated vector space of linear mappings,

$$\mathscr{M} = (M, S, +, \cdot) \quad M = \{A \mid \boldsymbol{A} = \begin{bmatrix} \boldsymbol{f}(\boldsymbol{u}_1) & \boldsymbol{f}(\boldsymbol{u}_2) & \ldots \end{bmatrix}\}.$$

The addition $\boldsymbol{C} = \boldsymbol{A} + \boldsymbol{B}$ and scaling $\boldsymbol{S} = a\boldsymbol{R}$ of matrices is given in terms of the matrix components by

$$c_{ij} = a_{ij} + b_{ij}, s_{ij} = ar_{\mathrm{ij}}.$$

1.2. Measurement of mappings

From the above it is apparent that linear mappings and matrices can also be considered as data, and a first step in analysis of such data is definition of functionals that would attach a single scalar label to each linear mapping of matrix. Of particular interest is the definition of a norm functional that characterizes in an appropriate sense the size of a linear mapping.

Consider first the case of finite matrices with real components $\boldsymbol{A} \in \mathbb{R}^{m\times n}$ that represent linear mappings between real vector spaces $\boldsymbol{f}: \mathbb{R}^m \longrightarrow \mathbb{R}^n$. The columns $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_n$ of $\boldsymbol{A} \in \mathbb{R}^{m\times n}$ could be placed into a single column vector $\boldsymbol{c}$ with mn components

$$\boldsymbol{c} = \begin{bmatrix} \boldsymbol{a}_1 \\ \vdots \\ \boldsymbol{a}_n \end{bmatrix}.$$

Subsequently the norm of the matrix $\boldsymbol{A}$ could be defined as the norm of the vector $\boldsymbol{c}$. An example of this approach is the Frobenius norm

$$\| \boldsymbol{A} \|_F = \| \boldsymbol{c} \|_2 = \left(\sum_{i=1}^{m} \sum_{j=1}^{n} | a_{ij} |^2 \right)^{1/2}.$$

A drawback of the above approach is that the structure of the matrix and its close relationship to a linear mapping is lost. A more useful characterization of the size of a mapping is to consider the amplification behavior of linear mapping. The motivation is readily understood starting from linear mappings between the reals $f: \mathbb{R} \longrightarrow \mathbb{R}$, that are of the form $f(x) = ax$. When given an argument of unit magnitude $|x| = 1$, the mapping returns a real number with magnitude $|a|$. For mappings $\boldsymbol{f}: \mathbb{R}^2 \longrightarrow \mathbb{R}^2$ within the plane, arguments that satisfy $\| \boldsymbol{x} \|_2 = 1$ are on the unit circle with components $\boldsymbol{x} = [\, \cos\theta \;\; \sin\theta \,]$ have images through $\boldsymbol{f}$ given analytically by

$$\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x} = \begin{bmatrix} \boldsymbol{a}_1 & \boldsymbol{a}_2 \end{bmatrix} \begin{bmatrix} \cos\theta \\ \sin\theta \end{bmatrix} = \cos\theta \boldsymbol{a}_1 + \sin\theta \boldsymbol{a}_2,$$

and correspond to ellipses.

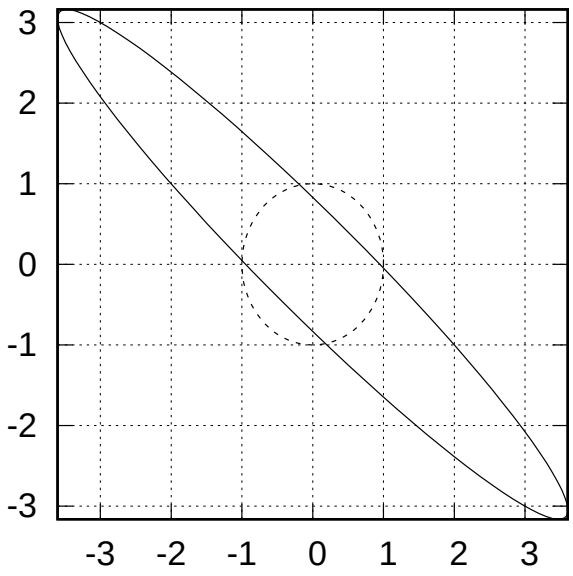


Figure 1. Mapping of unit circle by $\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x}$, $\boldsymbol{A} = \begin{bmatrix} 2 & 3 \\ -1 & -3 \end{bmatrix}$.

From the above the mapping associated $\boldsymbol{A}$ amplifies some directions more than others. This suggests a definition of the size of a matrix or a mapping by the maximal amplification unit norm vectors within the domain.

DEFINITION. *For vector spaces U, V with norms $\| \ \|_U : U \longrightarrow \mathbb{R}_+$, $\| \ \|_V : V \longrightarrow \mathbb{R}_+$, the induced norm of $\boldsymbol{f} : U \longrightarrow V$ is*

$$\| \boldsymbol{f} \| = \sup_{\|\boldsymbol{x}\|_U = 1} \| \boldsymbol{f}(\boldsymbol{x}) \|_V .$$

DEFINITION. *For vector spaces $\mathbb{R}^n, \mathbb{R}^m$ with norms $\| \ \|^{(n)} : U \longrightarrow \mathbb{R}_+$, $\| \ \|^{(m)} : V \longrightarrow \mathbb{R}_+$, the induced norm of matrix $\boldsymbol{A} \in \mathbb{R}^{m \times n}$ is*

$$\| \boldsymbol{A} \| = \sup_{\|\boldsymbol{x}\|^{(n)} = 1} \| \boldsymbol{A}\boldsymbol{x} \|^{(m)} .$$

In the above, any vector norm can be used within the domain and codomain.

2. The Singular Value Decomposition (SVD)

The fundamental theorem of linear algebra partitions the domain and codomain of a linear mapping $\boldsymbol{f} : U \longrightarrow V$. For real vectors spaces $U = \mathbb{R}^n$, $V = \mathbb{R}^m$ the partition properties are stated in terms of spaces of the associated matrix $\boldsymbol{A}$ as

$$C(\boldsymbol{A}) \oplus N(\boldsymbol{A}^T) = \mathbb{R}^m \quad C(\boldsymbol{A}) \perp N(\boldsymbol{A}^T) \quad C(\boldsymbol{A}^T) \oplus N(\boldsymbol{A}) = \mathbb{R}^n \quad C(\boldsymbol{A}^T) \perp N(\boldsymbol{A}) \ .$$

The dimension of the column and row spaces $r = \dim C(\boldsymbol{A}) = \dim C(\boldsymbol{A}^T)$ is the rank of the matrix, $n - r$ is the nullity of $\boldsymbol{A}$, and $m - r$ is the nullity of A^T. A infinite number of bases could be defined for the domain and codomain. It is of great theoretical and practical interest bases with properties that faciliatate insight or computation.

2.1. Orthogonal matrices

The above partitions of the domain and codomain are orthogonal, and suggest searching for orthogonal bases within these subspaces. Introduce a matrix representation for the bases

$$\boldsymbol{U} = \begin{bmatrix} \boldsymbol{u}_1 & \boldsymbol{u}_2 & \dots & \boldsymbol{u}_m \end{bmatrix} \in \mathbb{R}^{m \times m}, \boldsymbol{V} = \begin{bmatrix} \boldsymbol{v}_1 & \boldsymbol{v}_2 & \dots & \boldsymbol{v}_n \end{bmatrix} \in \mathbb{R}^{n \times n},$$

with $C(\boldsymbol{U}) = \mathbb{R}^m$ and $C(\boldsymbol{V}) = \mathbb{R}^n$. Orthogonality between columns $\boldsymbol{u}_i$, $\boldsymbol{u}_j$ for $i \neq j$ is expressed as $\boldsymbol{u}_i^T \boldsymbol{u}_j = 0$. For $i = j$, the inner product is positive $\boldsymbol{u}_i^T \boldsymbol{u}_i > 0$, and since scaling of the columns of $\boldsymbol{U}$ preserves the spanning property $C(\boldsymbol{U}) = \mathbb{R}^m$, it is convenient to impose $\boldsymbol{u}_i^T \boldsymbol{u}_i = 1$. Such behavior is concisely expressed as a matrix product

$$\boldsymbol{U}^T \boldsymbol{U} = \boldsymbol{I}_m,$$

with $\boldsymbol{I}_m$ the identity matrix in $\mathbb{R}^m$. Expanded in terms of the column vectors of $\boldsymbol{U}$ the first equality is

$$\begin{bmatrix} \boldsymbol{u}_1 & \boldsymbol{u}_2 & \dots & \boldsymbol{u}_m \end{bmatrix}^T \begin{bmatrix} \boldsymbol{u}_1 & \boldsymbol{u}_2 & \dots & \boldsymbol{u}_m \end{bmatrix} = \begin{bmatrix} \boldsymbol{u}_1^T \\ \boldsymbol{u}_2^T \\ \vdots \\ \boldsymbol{u}_m^T \end{bmatrix} \begin{bmatrix} \boldsymbol{u}_1 & \boldsymbol{u}_2 & \dots & \boldsymbol{u}_m \end{bmatrix} = \begin{bmatrix} \boldsymbol{u}_1^T \boldsymbol{u}_1 & \boldsymbol{u}_1^T \boldsymbol{u}_2 & \dots & \boldsymbol{u}_1^T \boldsymbol{u}_m \\ \boldsymbol{u}_2^T \boldsymbol{u}_1 & \boldsymbol{u}_2^T \boldsymbol{u}_2 & \dots & \boldsymbol{u}_2^T \boldsymbol{u}_m \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{u}_m^T \boldsymbol{u}_1 & \boldsymbol{u}_m^T \boldsymbol{u}_2 & \dots & \boldsymbol{u}_m^T \boldsymbol{u}_m \end{bmatrix} = \boldsymbol{I}_m .$$

It is useful to determine if a matrix $\boldsymbol{X}$ exists such that $\boldsymbol{UX} = \boldsymbol{I}_m$, or

$$\boldsymbol{UX} = \boldsymbol{U}\left[\begin{array}{cccc}\boldsymbol{x}_1 & \boldsymbol{x}_2 & \dots & \boldsymbol{x}_m\end{array}\right] = \left[\begin{array}{cccc}\boldsymbol{e}_1 & \boldsymbol{e}_2 & \dots & \boldsymbol{e}_m\end{array}\right].$$

The columns of $\boldsymbol{X}$ are the coordinates of the column vectors of $\boldsymbol{I}_m$ in the basis $\boldsymbol{U}$, and can readily be determined

$$\boldsymbol{U}\boldsymbol{x}_j = \boldsymbol{e}_j \Longrightarrow \boldsymbol{U}^T\boldsymbol{U}\boldsymbol{x}_j = \boldsymbol{U}^T\boldsymbol{e}_j \Longrightarrow \boldsymbol{I}_m\boldsymbol{x}_j = \begin{bmatrix}\boldsymbol{u}_1^T \\ \boldsymbol{u}_2^T \\ \vdots \\ \boldsymbol{u}_m^T\end{bmatrix}\boldsymbol{e}_j \Longrightarrow \boldsymbol{x}_j = (\boldsymbol{U}^T)_j,$$

where $(\boldsymbol{U}^T)_j$ is the j^{th} column of $\boldsymbol{U}^T$, hence $\boldsymbol{X} = \boldsymbol{U}^T$, leading to

$$\boldsymbol{U}^T\boldsymbol{U} = \boldsymbol{I} = \boldsymbol{U}\boldsymbol{U}^T.$$

Note that the second equality

$$\left[\begin{array}{cccc}\boldsymbol{u}_1 & \boldsymbol{u}_2 & \dots & \boldsymbol{u}_m\end{array}\right]\left[\begin{array}{cccc}\boldsymbol{u}_1 & \boldsymbol{u}_2 & \dots & \boldsymbol{u}_m\end{array}\right]^T = \left[\begin{array}{cccc}\boldsymbol{u}_1 & \boldsymbol{u}_2 & \dots & \boldsymbol{u}_m\end{array}\right]\begin{bmatrix}\boldsymbol{u}_1^T \\ \boldsymbol{u}_2^T \\ \vdots \\ \boldsymbol{u}_m^T\end{bmatrix} = \boldsymbol{u}_1\boldsymbol{u}_1^T + \boldsymbol{u}_2\boldsymbol{u}_2^T + \cdots + \boldsymbol{u}_m\boldsymbol{u}_m^T = \boldsymbol{I}$$

acts as normalization condition on the matrices $\boldsymbol{U}_j = \boldsymbol{u}_j\boldsymbol{u}_j^T$.

DEFINITION. *A square matrix $\boldsymbol{U}$ is said to be orthogonal if $\boldsymbol{U}^T\boldsymbol{U} = \boldsymbol{U}\boldsymbol{U}^T = \boldsymbol{I}$.*

2.2. Intrinsic basis of a linear mapping

Given a linear mapping $\boldsymbol{f}: U \longrightarrow V$, expressed as $\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x}$, the simplest description of the action of $\boldsymbol{A}$ would be a simple scaling, as exemplified by $\boldsymbol{g}(\boldsymbol{x}) = a\boldsymbol{x}$ that has as its associated matrix $a\boldsymbol{I}$. Recall that specification of a vector is typically done in terms of the identity matrix $\boldsymbol{b} = \boldsymbol{I}\boldsymbol{b}$, but may be more insightfully given in some other basis $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{I}\boldsymbol{b}$. This suggests that especially useful bases for the domain and codomain would reduce the action of a linear mapping to scaling along orthogonal directions, and evaluate $\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}$ by first re-expressing $\boldsymbol{y}$ in another basis $\boldsymbol{U}$, $\boldsymbol{U}\boldsymbol{s} = \boldsymbol{I}\boldsymbol{y}$ and re-expressing $\boldsymbol{x}$ in another basis $\boldsymbol{V}$, $\boldsymbol{V}\boldsymbol{r} = \boldsymbol{I}\boldsymbol{x}$. The condition that the linear operator reduces to simple scaling in these new bases is expressed as $s_i = \sigma_i r_i$ for $i = 1, \dots, \min(m, n)$, with σ_i the scaling coefficients along each direction which can be expressed as a matrix vector product $\boldsymbol{s} = \boldsymbol{\Sigma}\boldsymbol{r}$, where $\boldsymbol{\Sigma} \in \mathbb{R}^{m\times n}$ is of the same dimensions as $\boldsymbol{A}$ and given by

$$\boldsymbol{\Sigma} = \begin{bmatrix}\sigma_1 & 0 & \dots & 0 & 0 & \dots & 0 \\ 0 & \sigma_2 & \dots & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & 0 & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma_r & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 0 & 0 & \dots & 0\end{bmatrix}.$$

Imposing the condition that $\boldsymbol{U}, \boldsymbol{V}$ are orthogonal leads to

$$\boldsymbol{U}\boldsymbol{s} = \boldsymbol{y} \Longrightarrow \boldsymbol{s} = \boldsymbol{U}^T\boldsymbol{y}, \boldsymbol{V}\boldsymbol{r} = \boldsymbol{x} \Longrightarrow \boldsymbol{r} = \boldsymbol{V}^T\boldsymbol{x},$$

which can be replaced into $\boldsymbol{s} = \boldsymbol{\Sigma}\boldsymbol{r}$ to obtain

$$\boldsymbol{U}^T\boldsymbol{y} = \boldsymbol{\Sigma}\boldsymbol{V}^T\boldsymbol{x} \Longrightarrow \boldsymbol{y} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T\boldsymbol{x}.$$

From the above the orthogonal bases $\boldsymbol{U}, \boldsymbol{V}$ and scaling coefficients $\boldsymbol{\Sigma}$ that are sought must satisfy $\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T$.

THEOREM. *Every matrix $\boldsymbol{A} \in \mathbb{R}^{m\times n}$ has a singular value decomposition (SVD)*

$$\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T,$$

with properties:

1. $\boldsymbol{U} \in \mathbb{R}^{m\times m}$ *is an orthogonal matrix,* $\boldsymbol{U}^T\boldsymbol{U} = \boldsymbol{I}_m$;
2. $\boldsymbol{V} \in \mathbb{R}^{m\times m}$ *is an orthogonal matrix,* $\boldsymbol{V}^T\boldsymbol{V} = \boldsymbol{I}_n$;
3. $\boldsymbol{\Sigma} \in \mathbb{R}^{m\times n}$ *is diagonal,* $\boldsymbol{\Sigma} = \text{diag}(\sigma_1, \ldots, \sigma_p)$, $p = \min(m, n)$, *and* $\sigma_1 \geqslant \sigma_2 \geqslant \cdots \geqslant \sigma_p \geqslant 0$.

Proof. *The proof of the SVD makes use of properties of the norm, concepts from analysis and complete induction. Adopting the 2-norm set* $\sigma_1 = \|A\|_2$,

$$\sigma_1 = \sup_{\|\boldsymbol{x}\|_2 = 1} \|\boldsymbol{A}\boldsymbol{x}\|_2.$$

The domain $\|\boldsymbol{x}\|_2 = 1$ *is compact (closed and bounded), and the extreme value theorem implies that* $\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x}$ *attains its maxima and minima, hence there must exist some vectors* $\boldsymbol{u}_1, \boldsymbol{v}_1$ *of unit norm such that* $\sigma_1\boldsymbol{u}_1 = \boldsymbol{A}\boldsymbol{v}_1 \Longrightarrow \sigma_1 = \boldsymbol{u}_1^T\boldsymbol{A}\boldsymbol{v}_1$. *Introduce orthogonal bases* $\boldsymbol{U}_1$, $\boldsymbol{V}_1$ *for* $\mathbb{R}^m, \mathbb{R}^n$ *whose first column vectors are* $\boldsymbol{u}_1, \boldsymbol{v}_1$, *and compute*

$$\boldsymbol{U}_1{}^T\boldsymbol{A}\boldsymbol{V}_1 = \begin{bmatrix} \boldsymbol{u}_1^T \\ \vdots \\ \boldsymbol{u}_m^T \end{bmatrix} \begin{bmatrix} \boldsymbol{A}\boldsymbol{v}_1 & \ldots & \boldsymbol{A}\boldsymbol{v}_n \end{bmatrix} = \begin{bmatrix} \sigma_1 & \boldsymbol{w}^T \\ \boldsymbol{0} & \boldsymbol{B} \end{bmatrix} = \boldsymbol{C}.$$

In the above $\boldsymbol{w}^T$ *is a row vector with* $n-1$ *components* $\boldsymbol{u}_1^T\boldsymbol{A}\boldsymbol{v}_j$, $j = 2, \ldots, n$, *and* $\boldsymbol{u}_i^T\boldsymbol{A}\boldsymbol{v}_1$ *must be zero for* $\boldsymbol{u}_1$ *to be the direction along which the maximum norm* $\|\boldsymbol{A}\boldsymbol{v}_1\|$ *is obtained. Introduce vectors*

$$\boldsymbol{y} = \begin{bmatrix} \sigma_1 \\ \boldsymbol{w} \end{bmatrix}, \boldsymbol{z} = \boldsymbol{C}\boldsymbol{y} = \begin{bmatrix} \sigma_1^2 + \boldsymbol{w}^T\boldsymbol{w} \\ \boldsymbol{B}\boldsymbol{w} \end{bmatrix},$$

and note that $\|\boldsymbol{z}\|_2 \geqslant \|\boldsymbol{y}\|_2^2 = \sigma_1^2 + \boldsymbol{w}^T\boldsymbol{w}$. *From* $\|\boldsymbol{U}_1{}^T\boldsymbol{A}\boldsymbol{V}_1\| = \|\boldsymbol{A}\| = \sigma_1 = \|\boldsymbol{C}\| \geqslant \sigma_1^2 + \boldsymbol{w}^T\boldsymbol{w}$ *it results that* $\boldsymbol{w} = \boldsymbol{0}$. *By induction, assume that* $\boldsymbol{B}$ *has a singular value decomposition,* $\boldsymbol{B} = \boldsymbol{U}_2\boldsymbol{\Sigma}_2\boldsymbol{V}_2^T$, *such that*

$$\boldsymbol{U}_1{}^T\boldsymbol{A}\boldsymbol{V}_1 = \begin{bmatrix} \sigma_1 & \boldsymbol{0}^T \\ \boldsymbol{0} & \boldsymbol{U}_2\boldsymbol{\Sigma}_2\boldsymbol{V}_2^T \end{bmatrix} = \begin{bmatrix} 1 & \boldsymbol{0}^T \\ \boldsymbol{0} & \boldsymbol{U}_2 \end{bmatrix} \begin{bmatrix} \sigma_1 & \boldsymbol{0}^T \\ \boldsymbol{0} & \boldsymbol{\Sigma}_2 \end{bmatrix} \begin{bmatrix} 1 & \boldsymbol{0}^T \\ \boldsymbol{0} & \boldsymbol{V}_2^T \end{bmatrix},$$

and the orthogonal matrices arising in the singular value decomposition of $\boldsymbol{A}$ *are*

$$\boldsymbol{U} = \boldsymbol{U}_1 \begin{bmatrix} 1 & \boldsymbol{0}^T \\ \boldsymbol{0} & \boldsymbol{U}_2 \end{bmatrix}, \boldsymbol{V}^T = \begin{bmatrix} 1 & \boldsymbol{0}^T \\ \boldsymbol{0} & \boldsymbol{V}_2^T \end{bmatrix} \boldsymbol{V}_1^T.$$

□

The scaling coefficients σ_j are called the *singular values* of $\boldsymbol{A}$. The columns of $\boldsymbol{U}$ are called the *left singular vectors*, and those of $\boldsymbol{V}$ are called the *right singular vectors*.

The fact that the scaling coefficients are norms of $\boldsymbol{A}$ and submatrices of $\boldsymbol{A}$, $\sigma_1 = \|\boldsymbol{A}\|$, is crucial importance in applications. Carrying out computation of the matrix products

$$\boldsymbol{A} = \begin{bmatrix} \boldsymbol{u}_1 & \boldsymbol{u}_2 & \dots & \boldsymbol{u}_r & \boldsymbol{u}_{r+1} & \dots & \boldsymbol{u}_m \end{bmatrix} \begin{bmatrix} \sigma_1 & 0 & \dots & 0 & 0 & \dots & 0 \\ 0 & \sigma_2 & \dots & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & 0 & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma_r & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 0 & 0 & \dots & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{v}_1^T \\ \boldsymbol{v}_2^T \\ \vdots \\ \boldsymbol{v}_r^T \\ \vdots \\ \boldsymbol{v}_n^T \end{bmatrix} = \begin{bmatrix} \boldsymbol{u}_1 & \boldsymbol{u}_2 & \dots & \boldsymbol{u}_r & \boldsymbol{u}_{r+1} & \dots & \boldsymbol{u}_m \end{bmatrix} \begin{bmatrix} \sigma_1 \boldsymbol{v}_1^T \\ \sigma_2 \boldsymbol{v}_2^T \\ \vdots \\ \sigma_r \boldsymbol{v}_r^T \\ \vdots \\ 0 \end{bmatrix}$$

leads to a representation of $\boldsymbol{A}$ as a sum

$$\boldsymbol{A} = \sum_{i=1}^{r} \sigma_i \boldsymbol{u}_i \boldsymbol{v}_i^T, r \leqslant \min(m, n).$$

Each product $\boldsymbol{u}_i \boldsymbol{v}_i^T$ is a matrix of rank one, and is called a rank-one update. Truncation of the above sum to p terms leads to an approximation of $\boldsymbol{A}$

$$\boldsymbol{A} \cong \boldsymbol{A}_p = \sum_{i=1}^{p} \sigma_i \boldsymbol{u}_i \boldsymbol{v}_i^T.$$

In very many cases the singular values exhibit rapid, exponential decay, $\sigma_1 \gg \sigma_2 \gg \cdots$, such that the approximation above is an accurate representation of the matrix $\boldsymbol{A}$.

Figure 3.2. Successive SVD approximations of Frida Kahlo's (1907-1954) painting, *Portrait of a Lady in White* (1929), with $k = 10, 20, 40$ rank-one updates.

2.3. SVD solution of linear algebra problems

The SVD can be used to solve common problems within linear algebra.

Change of coordinates. To change from vector coordinates $\boldsymbol{b}$ in the canonical basis $\boldsymbol{I} \in \mathbb{R}^{m \times m}$ to coordinates $\boldsymbol{x}$ in some other basis $\boldsymbol{A} \in \mathbb{R}^{m \times m}$, a solution to the equation $\boldsymbol{Ib} = \boldsymbol{Ax}$ can be found by the following steps.

1. Compute the SVD, $\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T = \boldsymbol{A}$;
2. Find the coordinates of $\boldsymbol{b}$ in the orthogonal basis $\boldsymbol{U}$, $\boldsymbol{c} = \boldsymbol{U}^T\boldsymbol{b}$;
3. Scale the coordinates of $\boldsymbol{c}$ by the inverse of the singular values $y_i = c_i/\sigma_i$, $i = 1, \ldots, m$, such that $\Sigma\, \boldsymbol{y} = \boldsymbol{c}$ is satisfied;
4. Find the coordinates of $\boldsymbol{y}$ in basis $\boldsymbol{V}^T$, $\boldsymbol{x} = \boldsymbol{V}\boldsymbol{y}$.

Best 2-norm approximation. In the above $\boldsymbol{A}$ was assumed to be a basis, hence $r = \text{rank}(\boldsymbol{A}) = m$. If columns of $\boldsymbol{A}$ do not form a basis, $r < m$, then $\boldsymbol{b} \in \mathbb{R}^m$ might not be reachable by linear combinations within $C(\boldsymbol{A})$. The closest vector to $\boldsymbol{b}$ in the norm is however found by the same steps, with the simple modification that in Step 3, the scaling is carried out only for non-zero singular values, $y_i = c_i/\sigma_i$, $i = 1, \ldots, r$.

The pseudo-inverse. From the above, finding either the solution of $\boldsymbol{Ax} = \boldsymbol{Ib}$ or the best approximation possible if $\boldsymbol{A}$ is not of full rank, can be written as a sequence of matrix multiplications using the SVD

$$(\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T)\,\boldsymbol{x} = \boldsymbol{b} \Longrightarrow \boldsymbol{U}\,(\boldsymbol{\Sigma}\boldsymbol{V}^T\boldsymbol{x}) = \boldsymbol{b} \Longrightarrow (\boldsymbol{\Sigma}\boldsymbol{V}^T\boldsymbol{x}) = \boldsymbol{U}^T\boldsymbol{b} \Longrightarrow \boldsymbol{V}^T\boldsymbol{x} = \boldsymbol{\Sigma}^+\boldsymbol{U}^T\boldsymbol{b} \Longrightarrow \boldsymbol{x} = \boldsymbol{V}\boldsymbol{\Sigma}^+\boldsymbol{U}^T\boldsymbol{b},$$

where the matrix $\boldsymbol{\Sigma}^+ \in \mathbb{R}^{n \times m}$ (notice the inversion of dimensions) is defined as a matrix with elements σ_i^{-1} on the diagonal, and is called the pseudo-inverse of $\boldsymbol{\Sigma}$. Similarly the matrix

$$\boldsymbol{A}^+ = \boldsymbol{V}\boldsymbol{\Sigma}^+\boldsymbol{U}^T$$

that allows stating the solution of $\boldsymbol{Ax} = \boldsymbol{b}$ simply as $\boldsymbol{x} = \boldsymbol{A}^+\boldsymbol{b}$ is called the *pseudo-inverse* of $\boldsymbol{A}$. Note that in practice $\boldsymbol{A}^+$ is not explicitly formed. Rather the notation $\boldsymbol{A}^+$ is simply a concise reference to carrying out steps 1-4 above.

CHAPTER 4

LEAST SQUARES

DATA COMPRESSION

A typical scenario in many sciences is acquisition of m numbers to describe some object that is understood to actually require only $n \ll m$ parameters. For example, m voltage measurements u_i of an alternating current could readily be reduced to three parameters, the amplitude, phase and frequency $u(t) = a\sin(\omega t + \varphi)$. Very often a simple first-degree polynomial approximation $y = ax + b$ is sought for a large data set $D = \{(x_i, y_i), i = 1, \ldots, m\}$. All of these are instances of data compression, a problem that can be solved in a linear algebra framework.

1. Projection

Consider a partition of a vector space U into orthogonal subspaces $U = V \oplus W$, $V = W^{\perp}$, $W = V^{\perp}$. Within the typical scenario described above $U = \mathbb{R}^m$, $V \subset \mathbb{R}^m$, $W \subset \mathbb{R}^m$, $\dim V = n$, $\dim W = m - n$. If $\boldsymbol{V} = [\ \boldsymbol{v}_1\ \ \ldots\ \ \boldsymbol{v}_n\ ] \in \mathbb{R}^{m\times n}$ is a basis for V and $\boldsymbol{W} = [\ \boldsymbol{w}_1\ \ \ldots\ \ \boldsymbol{w}_{m-n}\ ] \in \mathbb{R}^{m\times(m-n)}$ is a basis for W, then $\boldsymbol{U} = [\ \boldsymbol{v}_1\ \ \ldots\ \ \boldsymbol{v}_n\ \ \boldsymbol{w}_1\ \ \ldots\ \ \boldsymbol{w}_{m-n}\ ]$ is a basis for U. Even though the matrices $\boldsymbol{V}, \boldsymbol{W}$ are not necessarily square, they are said to be orthogonal, in the sense that all columns are of unit norm and orthogonal to one another. Computation of the matrix product $\boldsymbol{V}^T\boldsymbol{V}$ leads to the formation of the identity matrix within $\mathbb{R}^n$

$$\boldsymbol{V}^T\boldsymbol{V} = \begin{bmatrix} \boldsymbol{v}_1^T \\ \boldsymbol{v}_2^T \\ \vdots \\ \boldsymbol{v}_n^T \end{bmatrix} [\ \boldsymbol{v}_1\ \ \boldsymbol{v}_2\ \ \ldots\ \ \boldsymbol{v}_n\ ] = \begin{bmatrix} \boldsymbol{v}_1^T\boldsymbol{v}_1 & \boldsymbol{v}_1^T\boldsymbol{v}_2 & \ldots & \boldsymbol{v}_1^T\boldsymbol{v}_n \\ \boldsymbol{v}_2^T\boldsymbol{v}_1 & \boldsymbol{v}_2^T\boldsymbol{v}_2 & \ldots & \boldsymbol{v}_2^T\boldsymbol{v}_n \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{v}_n^T\boldsymbol{v}_1 & \boldsymbol{v}_n^T\boldsymbol{v}_2 & \ldots & \boldsymbol{v}_n^T\boldsymbol{v}_n \end{bmatrix} = \boldsymbol{I}_n.$$

Similarly, $\boldsymbol{W}^T\boldsymbol{W} = \boldsymbol{I}_{m-n}$. Whereas for the square orthogonal matrix $\boldsymbol{U}$ multiplication both on the left and the right by its transpose leads to the formation of the identity matrix

$$\boldsymbol{U}^T\boldsymbol{U} = \boldsymbol{U}\boldsymbol{U}^T = \boldsymbol{I}_m,$$

the same operations applied to rectangular orthogonal matrices lead to different results

$$\boldsymbol{V}^T\boldsymbol{V} = \boldsymbol{I}_n,\ \boldsymbol{V}\boldsymbol{V}^T = [\ \boldsymbol{v}_1\ \ \boldsymbol{v}_2\ \ \ldots\ \ \boldsymbol{v}_n\ ] \begin{bmatrix} \boldsymbol{v}_1^T \\ \boldsymbol{v}_2^T \\ \vdots \\ \boldsymbol{v}_n^T \end{bmatrix} = \sum_{i=1}^{n} \boldsymbol{v}_i\boldsymbol{v}_i^T,\ \mathrm{rank}(\boldsymbol{v}_i\boldsymbol{v}_i^T) = 1$$

A simple example is provided by taking $\boldsymbol{V} = \boldsymbol{I}_{m,n}$, the first n columns of the identity matrix in which case

$$\boldsymbol{V}\boldsymbol{V}^T = \sum_{i=1}^{n} \boldsymbol{e}_i\boldsymbol{e}_i^T = \begin{bmatrix} \boldsymbol{I}_n & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} \end{bmatrix} \in \mathbb{R}^{m\times m}.$$

Applying $\boldsymbol{P} = \boldsymbol{V}\boldsymbol{V}^T$ to some vector $\boldsymbol{b} \in \mathbb{R}^m$ leads to a vector $\boldsymbol{r} = \boldsymbol{P}\boldsymbol{b}$ whose first n components are those of $\boldsymbol{b}$, and the remaining $m-n$ are zero. The subtraction $\boldsymbol{b} - \boldsymbol{r}$ leads to a new vector $\boldsymbol{s} = (\boldsymbol{I} - \boldsymbol{P})\boldsymbol{b}$ that has the first components equal to zero, and the remaining $m-n$ the same as those of $\boldsymbol{b}$. Such operations are referred to as *projections*, and for $\boldsymbol{V} = \boldsymbol{I}_{m,n}$ correspond to projection onto the span$\{\boldsymbol{e}_1, \ldots, \boldsymbol{e}_n\}$.

```
octave] I4=eye(5); V=I4(:,1:2); P=V*V'; Q=I4-P;
        b=rand(5,1); r=P*b; s=Q*b; disp([P b r s])
   1.00000   0.00000   0.00000   0.00000   0.00000   0.42253   0.42253   0.00000
   0.00000   1.00000   0.00000   0.00000   0.00000   0.95900   0.95900   0.00000
   0.00000   0.00000   0.00000   0.00000   0.00000   0.41781   0.00000   0.41781
   0.00000   0.00000   0.00000   0.00000   0.00000   0.45744   0.00000   0.45744
   0.00000   0.00000   0.00000   0.00000   0.00000   0.49784   0.00000   0.49784
octave]
```

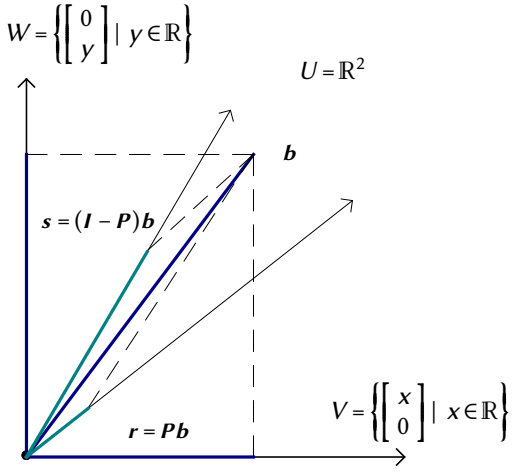


Figure 4.1. Projection in $\mathbb{R}^2$. The vectors $\boldsymbol{r}, \boldsymbol{s} \in \mathbb{R}^2$ have two components, but could be expressed through scaling of $\boldsymbol{e}_1, \boldsymbol{e}_2$.

Returning to the general case, the orthogonal matrices $\boldsymbol{U} \in \mathbb{R}^{m \times m}$, $\boldsymbol{V} \in \mathbb{R}^{m \times n}$, $\boldsymbol{W} \in \mathbb{R}^{m \times (m-n)}$ are associated with linear mappings $\boldsymbol{b} = \boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{U}\boldsymbol{x}$, $\boldsymbol{r} = \boldsymbol{g}(\boldsymbol{b}) = \boldsymbol{P}\boldsymbol{b}$, $\boldsymbol{s} = \boldsymbol{h}(\boldsymbol{b}) = (\boldsymbol{I} - \boldsymbol{P})\,\boldsymbol{b}$. The mapping $\boldsymbol{f}$ gives the components in the $\boldsymbol{I}$ basis of a vector whose components in the $\boldsymbol{U}$ basis are $\boldsymbol{x}$. The mappings $\boldsymbol{g}, \boldsymbol{h}$ project a vector onto span$\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_n\}$, span$\{\boldsymbol{w}_1, \ldots, \boldsymbol{w}_{m-n}\}$, respectively. When $\boldsymbol{V}, \boldsymbol{W}$ are orthogonal matrices the projections are also orthogonal $\boldsymbol{r} \perp \boldsymbol{s}$. Projection can also be carried out onto nonorthogonal spanning sets, but the process is fraught with possible error, especially when the angle between basis vectors is small, and will be avoided henceforth.

Notice that projection of a vector already in the spanning set simply returns the same vector, which leads to a general definition.

DEFINITION. *The mapping is called a projection if $\boldsymbol{f} \circ \boldsymbol{f} = \boldsymbol{f}$, or if for any $\boldsymbol{u} \in U$, $\boldsymbol{f}(\boldsymbol{f}(\boldsymbol{u})) = \boldsymbol{f}(\boldsymbol{u})$. With $\boldsymbol{P}$ the matrix associated $\boldsymbol{f}$, a projection matrix satisfies $\boldsymbol{P}^2 = \boldsymbol{P}$.*

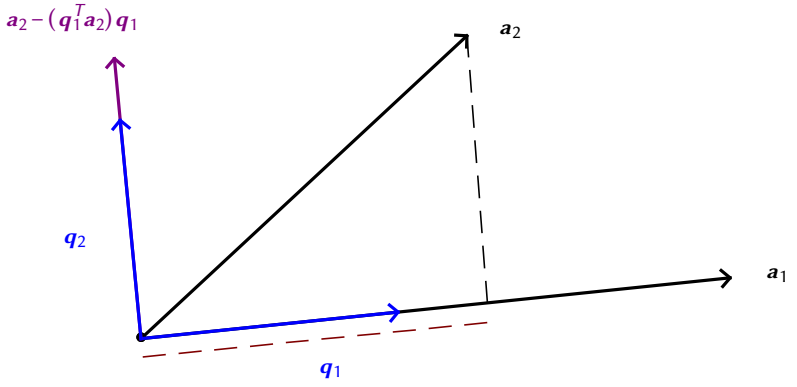
$$\boldsymbol{P} = \boldsymbol{V}\boldsymbol{V}^T$$

$$\boldsymbol{P}^2 = \boldsymbol{P}\boldsymbol{P} = \boldsymbol{V}\boldsymbol{V}^T\boldsymbol{V}\boldsymbol{V}^T = \boldsymbol{V}\left(\boldsymbol{V}^T\boldsymbol{V}\right)\boldsymbol{V}^T = \boldsymbol{V}\boldsymbol{I}\boldsymbol{V}^T = \boldsymbol{V}\boldsymbol{V}^T = \boldsymbol{P}$$

2. Gram-Schmidt

Orthonormal vector sets $\{\boldsymbol{q}_1,..., \boldsymbol{q}_n\}$ are of the greatest practical utility, leading to the question of whether some such a set can be obtained from an arbitrary set of vectors $\{\boldsymbol{a}_1,\ldots,\boldsymbol{a}_n\}$. This is possible for independent vectors, through what is known as the Gram-Schmidt algorithm

1. Start with an arbitrary direction $\boldsymbol{a}_1$
2. Divide by its norm to obtain a unit-norm vector $\boldsymbol{q}_1 = \boldsymbol{a}_1 / \|\boldsymbol{a}_1\|$
3. Choose another direction $\boldsymbol{a}_2$
4. Subtract off its component along previous direction(s) $\boldsymbol{a}_2 - (\boldsymbol{q}_1^T \boldsymbol{a}_2)\boldsymbol{q}_1$
5. Divide by norm $\boldsymbol{q}_2 = (\boldsymbol{a}_2 - (\boldsymbol{q}_1^T \boldsymbol{a}_2)\boldsymbol{q}_1) / \|\boldsymbol{a}_2 - (\boldsymbol{q}_1^T \boldsymbol{a}_2)\boldsymbol{q}_1\|$
6. Repeat the above



$$\boldsymbol{P}_1 \boldsymbol{a}_2 = (\boldsymbol{q}_1 \, \boldsymbol{q}_1^T)\boldsymbol{a}_2 = \boldsymbol{q}_1 (\boldsymbol{q}_1^T \boldsymbol{a}_2) = (\boldsymbol{q}_1^T \boldsymbol{a}_2) \, \boldsymbol{q}_1$$

The above geometrical description can be expressed in terms of matrix operations as

$$\boldsymbol{A} = \begin{pmatrix} \boldsymbol{a}_1 & \boldsymbol{a}_2 & \ldots & \boldsymbol{a}_n \end{pmatrix} = \begin{pmatrix} \boldsymbol{q}_1 & \boldsymbol{q}_2 & \ldots & \boldsymbol{q}_n \end{pmatrix} \begin{pmatrix} r_{11} & r_{12} & r_{13} & \ldots & r_{1n} \\ 0 & r_{22} & r_{23} & \ldots & r_{2n} \\ 0 & 0 & r_{33} & \ldots & r_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & \ldots & r_{mn} \end{pmatrix} = \boldsymbol{QR},$$

equivalent to the system

$$\begin{cases} \boldsymbol{a}_1 = r_{11}\boldsymbol{q}_1 \\ \boldsymbol{a}_2 = r_{12}\boldsymbol{q}_1 + r_{22}\boldsymbol{q}_2 \\ \vdots \\ \boldsymbol{a}_n = r_{1n}\boldsymbol{q}_1 + r_{2n}\boldsymbol{q}_2 + \ldots + r_{nn}\boldsymbol{q}_n \end{cases}.$$

The system is easily solved by *forward substitution* resulting in what is known as the (modified) *Gram-Schmidt algorithm*, transcribed below both in pseudo-code and in Octave.

Algorithm (Gram-Schmidt)

Given n vectors $\boldsymbol{a}_1,\ldots,\boldsymbol{a}_n$
Initialize $\boldsymbol{q}_1=\boldsymbol{a}_1,..,\boldsymbol{q}_n=\boldsymbol{a}_n$, $\boldsymbol{R}=\boldsymbol{I}_n$
for $i=1$ to n
  $r_{ii}=(\boldsymbol{q}_i^T\boldsymbol{q}_i)^{1/2}$
  if $r_{ii}<\epsilon$ break;
  $\boldsymbol{q}_i=\boldsymbol{q}_i/r_{ii}$
  for $j=i+1$ to n
    $r_{ij}=\boldsymbol{q}_i^T\boldsymbol{a}_j$; $\boldsymbol{q}_j=\boldsymbol{q}_j-r_{ij}\boldsymbol{q}_i$
  end
end
return $\boldsymbol{Q},\boldsymbol{R}$

```
octave] function [Q,R] = mgs(A)
          [m,n]=size(A); Q=A; R=eye(n);
          for i=1:n
            R(i,i) = sqrt(Q(:,i)'*Q(:,i));
            if (R(i,i)<eps) break;
            Q(:,i) = Q(:,i)/R(i,i);
            for j=i+1:n
              R(i,j) = Q(:,i)'*A(:,j);
              Q(:,j) = Q(:,j) - R(i,j)*Q(:,i);
            end;
          end;
        end
octave]
```

Note that the normalization condition $\|\boldsymbol{q}_{ii}\|=1$ is satisifed by two values $\pm r_{ii}$, so results from the above implementation might give orthogonal vectors $\boldsymbol{q}_1,\ldots,\boldsymbol{q}_n$ of different orientations than those returned by the Octave qr function. The implementation provided by computational packages such as Octave contain many refinements of the basic algorithm and it's usually preferable to use these in applications.

```
octave] A=rand(4); [Q,R]=mgs(A); disp([Q R])
   0.82757  -0.25921  -0.49326   0.06802   0.83553   0.64827   1.24651   1.05301
   0.19408   0.53127   0.15805   0.80939   0.00000   0.93177   0.82700   0.87551
   0.22006   0.79553  -0.12477  -0.55058   0.00000   0.00000   0.38433  -0.20336
   0.47857  -0.13302   0.84625  -0.19270   0.00000   0.00000   0.00000   0.42469
octave] [Q1,R1]=qr(A); disp([Q1 R1])
  -0.82757   0.25921  -0.49326  -0.06802  -0.83553  -0.64827  -1.24651  -1.05301
  -0.19408  -0.53127   0.15805  -0.80939   0.00000  -0.93177  -0.82700  -0.87551
  -0.22006  -0.79553  -0.12477   0.55058   0.00000   0.00000   0.38433  -0.20336
  -0.47857   0.13302   0.84625   0.19270   0.00000   0.00000   0.00000  -0.42469
octave] disp([norm(A-Q*R) norm(A-Q1*R1)])
   1.1102e-16   8.0390e-16
octave]
```

By analogy to arithmetic and polynomial algebra, the Gram-Schmidt algorithm furnishes a *factorization*

$$\boldsymbol{QR}=\boldsymbol{A}$$

with $\boldsymbol{Q}\in\mathbb{R}^{m\times n}$ with orthonormal columns and $\boldsymbol{R}\in\mathbb{R}^{n\times n}$ an upper triangular matrix, known as the QR-factorization. Since the column vectors within $\boldsymbol{Q}$ were obtained through linear combinations of the column vectors of $\boldsymbol{A}$ we have

$$C(\boldsymbol{A})=C(\boldsymbol{Q})\neq C(\boldsymbol{R})$$

$$\boldsymbol{AX}=\boldsymbol{B},\boldsymbol{A}\left[\begin{array}{ccc}\boldsymbol{x}_1 & \ldots & \boldsymbol{x}_n\end{array}\right]=\left[\begin{array}{ccc}\boldsymbol{Ax}_1 & \ldots & \boldsymbol{Ax}_n\end{array}\right].$$

The QR-factorization can be used to solve basic problems within linear algebra.

3. QR solution of linear algebra problems

3.1. Transformation of coordinates

Recall that when given a vector $\boldsymbol{b}\in\mathbb{R}^m$, an implicit basis is assumed, the canonical basis given by the column vectors of the identity matrix $\boldsymbol{I}\in\mathbb{R}^{m\times m}$. The coordinates $\boldsymbol{x}$ in another basis $\boldsymbol{A}\in\mathbb{R}^{m\times m}$ can be found by solving the equation

$$\boldsymbol{Ib}=\boldsymbol{b}=\boldsymbol{Ax},$$

by an intermediate change of coordinates to the orthogonal basis $\boldsymbol{Q}$. Since the basis $\boldsymbol{Q}$ is orthogonal the relation $\boldsymbol{Q}^T\boldsymbol{Q}=\boldsymbol{I}$ holds, and changes of coordinates from $\boldsymbol{I}$ to $\boldsymbol{Q}$, $\boldsymbol{Qc}=\boldsymbol{b}$, are easily computed $\boldsymbol{c}=\boldsymbol{Q}^T\boldsymbol{b}$. Since matrix multiplication is associative

$$\boldsymbol{b}=\boldsymbol{Ax}=(\boldsymbol{QR})\boldsymbol{x}=\boldsymbol{Q}\,(\boldsymbol{Rx}),$$

the relations $\boldsymbol{Rx}=\boldsymbol{Q}^T\boldsymbol{b}=\boldsymbol{c}$ are obtained, stating that $\boldsymbol{x}$ also contains the coordinates of $\boldsymbol{c}$ in the basis $\boldsymbol{R}$. The three steps are:

1. Compute the QR-factorization, $\boldsymbol{QR}=\boldsymbol{A}$;
2. Find the coordinates of $\boldsymbol{b}$ in the orthogonal basis $\boldsymbol{Q}$, $\boldsymbol{c}=\boldsymbol{Q}^T\boldsymbol{b}$;
3. Find the coordinates of $\boldsymbol{x}$ in basis $\boldsymbol{R}$, $\boldsymbol{Rx}=\boldsymbol{c}$.

Since $\boldsymbol{R}$ is upper-triangular,

$$\begin{pmatrix} r_{11} & r_{12} & r_{13} & \dots & r_{1m} \\ 0 & r_{22} & r_{23} & \dots & r_{2m} \\ 0 & 0 & r_{33} & \dots & r_{3m} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \dots & r_{mm} \end{pmatrix}\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{m-1} \\ x_m \end{bmatrix}=\begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_{m-1} \\ c_m \end{bmatrix}$$

the coordinates of $\boldsymbol{c}$ in the $\boldsymbol{R}$ basis are easily found by *back substitution*.

Algorithm (Back substitution)

Given R upper-triangular, vectors $\boldsymbol{c}$
for $i=m$ down to 1
  if $r_{ii}<\epsilon$ break;
  $x_i=c_i/r_{ii}$
  for $j=i$-1 down to 1
    $c_j=c_j-r_{ji}x_i$
  end
end
return $\boldsymbol{x}$

```
octave] function x=bcks(R,c)
         [m,n]=size(R); x=zeros(m,1);
         for i=m:-1:1
           x(i) = c(i)/R(i,i);
           for j=i-1:-1:1
             c(j) = c(j) - R(j,i)*x(i);
           end;
         end;
       end
octave]
```

The above operations are carried out in the background by the Octave backslash operation `A\b` to solve `A*x=b`, inspired by the scalar mnemonic $ax = b \Longrightarrow x = (1/a)\, b$. Again, many additional refinements of the basic algorithm argue for using the built-in Octave functions, even though the above implementations can be verified as correct.

```
octave] xex=rand(4,1); b=A*xex; [Q,R]=mgs(A); c=Q'*b; x=bcks(R,c); xO=A\b;
octave] disp([xex x xO])
   0.96838   0.96838   0.96838
   0.31829   0.31829   0.31829
   0.58529   0.58529   0.58529
   0.38250   0.38250   0.38250
octave]
```

3.2. General orthogonal bases

The above approch for the real vector space $\mathscr{R}_m$ can be used to determine orthogonal bases for any other vector space by appropriate modification of the scalar product. For example, within the space of smooth functions $C^\infty[-1, 1]$ that can differentiated an arbitrary number of times, the Taylor series

$$f(x) = f(0)\cdot 1 + f'(0)\cdot x + \tfrac{1}{2} f''(0)\cdot x^2 + \cdots + \tfrac{1}{n!} f^{(n)}(0)\cdot x^n + \cdots +$$

is seen to be a linear combination of the monomial basis $\boldsymbol{M} = \begin{bmatrix} 1 & x & x^2 & \dots \end{bmatrix}$ with scaling coefficients $\left\{ f(0), f'(0), \tfrac{1}{2} f''(0), \dots \right\}$. The scalar product

$$(f, g) = \int_{-1}^{1} f(x)\, g(x)\, \mathrm{d}x$$

can be seen as the extension to the $[-1, 1]$ continuum of a the vector dot product. Orthogonalization of the monomial basis with the above scalar product leads to the definition of another family of polynomials, known as the Legendre polynomials

$$Q_0(x) = \left(\tfrac{1}{2}\right)^{1/2}\cdot 1,\; Q_1(x) = \left(\tfrac{3}{2}\right)^{1/2}\cdot x,\; Q_2(x) = \left(\tfrac{5}{8}\right)^{1/2}\cdot (3x^2 - 1),\; Q_4(x) = \left(\tfrac{7}{8}\right)^{1/2}\cdot (5x^3 - 3x), \dots .$$

The Legendre polynomials are usually given with a different scaling such that $P_k(1) = 1$, rather than the unit norm condition $\| Q_k \| = (Q_k, Q_k)^{1/2} = 1$. The above results can be recovered by sampling of the interval $[-1, 1]$ at points $x_i = (i-1)\, h - 1$, $h = 2/(m-1)$, $i = 1, \dots, m$, by approximation of the integral by a Riemann sum

$$\int_{-1}^{1} f(x)\, L_j(x)\, \mathrm{d}x \cong h \sum_{i=1}^{m} f(x_i) L_j(x_i) = h\, \boldsymbol{f}^T \boldsymbol{L}_j .$$

```
octave] m=50; h=2/(m-1); x=(-1:h:1)'; M=[x.^0 x.^1 x.^2 x.^3 x.^4]; [Q,R]=mgs(M);
        S=diag(1./Q(m,:)); P=Q*S; sc=[-1 1 -1 1];
        figure(1); plot(x,M(:,1),x,M(:,2),x,M(:,3),x,M(:,4)); axis(sc); grid on;
        figure(2); plot(x,P(:,1),x,P(:,2),x,P(:,3),x,P(:,4)); axis(sc); grid on;
octave]
```

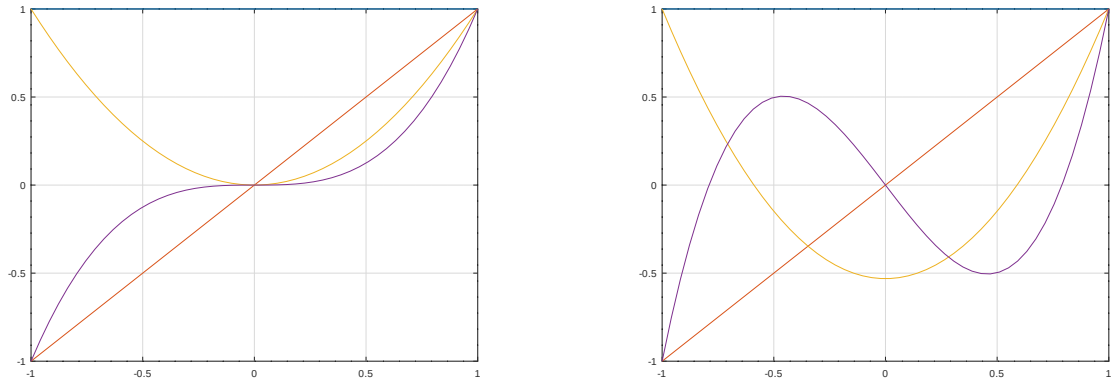


Figure 4.2. Comparison of monomial basis (left) to Legendre polynomial basis (right). The "resolution" of $P_3(x)$ can be interpreted as the number of crossings of the $y=0$ ordinate axis, and is greater than that of the corresponding monomial x^3.

3.3. Least squares

The approach to compressing data $D=\{(x_i,y_i)\mid i=1,\dots,m\}$ suggested by calculus concepts is to form the sum of squared differences between $y(x_i)$ and y_i, for example for $y(x)=a_0+a_1x$ when carrying out linear regression,

$$S(a_0,a_1)=\sum_{i=1}^{m}(y(x_i)-y_i)^2=\sum_{i=1}^{m}(a_0+a_1x_i-y_i)^2$$

and seek (a_0,a_1) that minimize $S(a_0,a_1)$. The function $S(a_0,a_1)\geqslant 0$ can be thought of as the height of a surface above the a_0a_1 plane, and the gradient ∇S is defined as a vector in the direction of steepest slope. When at some point on the surface if the gradient is different from the zero vector $\nabla S\neq\mathbf{0}$, travel in the direction of the gradient would increase the height, and travel in the opposite direction would decrease the height. The minimal value of S would be attained when no local travel could decrease the function value, which is known as stationarity condition, stated as $\nabla S=0$. Applying this to determining the coefficients (a_0,a_1) of a linear regression leads to the equations

$$\frac{\partial S}{\partial a_0}=0\Longrightarrow 2\sum_{i=1}^{m}(a_0+a_1x_i-y_i)=0\Longleftrightarrow ma_0+\left(\sum_{i=1}^{m}x_i\right)a_1=\sum_{i=1}^{m}y_i,$$

$$\frac{\partial S}{\partial a_1}=0\Longrightarrow 2\sum_{i=1}^{m}(a_0+a_1x_i-y_i)x_i=0\Longleftrightarrow\left(\sum_{i=1}^{m}x_i\right)a_0+\left(\sum_{i=1}^{m}x_i^2\right)a_1=\sum_{i=1}^{m}x_iy_i.$$

The above calculations can become tedious, and do not illuminate the geometrical essence of the calculation, which can be brought out by reformulation in terms of a matrix-vector product that highlights the particular linear combination that is sought in a liner regression. Form a vector of errors with components $e_i=y(x_i)-y_i$, which for linear regression is $y(x)=a_0+a_1x$. Recognize that $y(x_i)$ is a linear combination of 1 and x_i with coefficients a_0,a_1, or in vector form

$$\boldsymbol{e}=\begin{pmatrix}1 & x_1\\ \vdots & \vdots\\ 1 & x_m\end{pmatrix}\begin{pmatrix}a_0\\ a_1\end{pmatrix}-\boldsymbol{y}=(\,\mathbf{1}\;\;\boldsymbol{x}\,)\boldsymbol{a}-\boldsymbol{y}=\boldsymbol{A}\boldsymbol{a}-\boldsymbol{y}$$

The norm of the error vector $\|\boldsymbol{e}\|$ is smallest when $\boldsymbol{Aa}$ is as close as possible to $\boldsymbol{y}$. Since $\boldsymbol{Aa}$ is within the column space of $C(\boldsymbol{A})$, $\boldsymbol{Aa} \in C(\boldsymbol{A})$, the required condition is for $\boldsymbol{e}$ to be orthogonal to the column space

$$\boldsymbol{e} \perp C(\boldsymbol{A}) \Rightarrow \boldsymbol{A}^T\boldsymbol{e} = \begin{pmatrix} \mathbf{1}^T \\ \boldsymbol{x}^T \end{pmatrix}\boldsymbol{e} = \begin{pmatrix} \mathbf{1}^T\boldsymbol{e} \\ \boldsymbol{x}^T\boldsymbol{e} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} = \mathbf{0}$$

$$\boldsymbol{A}^T\boldsymbol{e} = \mathbf{0} \Leftrightarrow \boldsymbol{A}^T(\boldsymbol{Aa} - \boldsymbol{y}) = 0 \Leftrightarrow (\boldsymbol{A}^T\boldsymbol{A})\boldsymbol{a} = \boldsymbol{A}^T\boldsymbol{y} = \boldsymbol{b}.$$

The above is known as the normal system, with $\boldsymbol{N} = \boldsymbol{A}^T\boldsymbol{A}$ is the normal matrix. The system $\boldsymbol{Na} = \boldsymbol{b}$ can be interpreted as seeking the coordinates in the $\boldsymbol{N} = \boldsymbol{A}^T\boldsymbol{A}$ basis of the vector $\boldsymbol{b} = \boldsymbol{A}^T\boldsymbol{y}$. An example can be constructed by randomly perturbing a known function $y(x) = a_0 + a_1 x$ to simulate measurement noise and compare to the approximate $\tilde{\boldsymbol{a}}$ obtained by solving the normal system.

1. Generate some data on a line and perturb it by some random quantities

```
octave] m=100; x=(0:m-1)/m; a=[2; 3];
        a0=a(1); a1=a(2); yex=a0+a1*x; y=(yex+rand(1,m)-0.5)';
octave]
```

2. Form the matrices $\boldsymbol{A}$, $\boldsymbol{N} = \boldsymbol{A}^T\boldsymbol{A}$, vector $\boldsymbol{b} = \boldsymbol{A}^T\boldsymbol{y}$

```
octave] A=ones(m,2); A(:,2)=x(:); N=A'*A; b=A'*y;
octave]
```

3. Solve the system $\boldsymbol{Na} = \boldsymbol{b}$, and form the linear combination $\tilde{\boldsymbol{y}} = \boldsymbol{Aa}$ closest to $\boldsymbol{y}$

```
octave] atilde=N\b; disp([a atilde]);
   2.0000   2.0302
   3.0000   2.9628
octave]
```

The normal matrix basis $\boldsymbol{N} = \boldsymbol{A}^T\boldsymbol{A}$ can however be an ill-advised choice. Consider $\boldsymbol{A} \in \mathbb{R}^{2\times 2}$ given by

$$\boldsymbol{A} = \begin{bmatrix} \boldsymbol{a}_1 & \boldsymbol{a}_2 \end{bmatrix} = \begin{bmatrix} 1 & \cos\theta \\ 0 & \sin\theta \end{bmatrix},$$

where the first column vector is taken from the identity matrix $\boldsymbol{a}_1 = \boldsymbol{e}_1$, and second is the one obtained by rotating it with angle θ. If $\theta = \pi/2$, the normal matrix is orthogonal, $\boldsymbol{A}^T\boldsymbol{A} = \boldsymbol{I}$, but for small θ, $\boldsymbol{A}$ and $\boldsymbol{N} = \boldsymbol{A}^T\boldsymbol{A}$ are approximated as

$$\boldsymbol{A} \cong \begin{bmatrix} 1 & 1 \\ 0 & \theta \end{bmatrix}, \boldsymbol{N} = \begin{bmatrix} \boldsymbol{n}_1 & \boldsymbol{n}_2 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 0 & \theta^2 \end{bmatrix}.$$

When θ is small $\boldsymbol{a}_1, \boldsymbol{a}_2$ are almost colinear, and $\boldsymbol{n}_1, \boldsymbol{n}_2$ even more so. This can lead to amplification of small errors, but can be avoided by recognizing that the best approximation in the 2-norm is identical to the Euclidean concept of orthogonal projection. The orthogonal projector onto $C(\boldsymbol{A})$ is readily found by QR-factorization, and the steps to solve least squares become

1. Compute $\boldsymbol{QR} = \boldsymbol{A}$

2. The projection of y onto the column space of A is $z = QQ^T y$, and has coordinates $c = Q^T y$ in the orthogonal basis Q.

3. The same z can also obtained by linear combination of the columns of A, $z = Aa = QQ^T y$, and replacing A with its QR-factorization gives $QRa = Qc$, that leads to the system $Ra = c$, solved by back-substitution.

```
octave] [Q,R]=qr(A); c=Q'*y; aQR=R\c; disp([a atilde aQR])
   2.0000   2.0302   2.0302
   3.0000   2.9628   2.9628
octave]
```

The above procedure carried over to approximation by higher degree polynomials.

```
octave] m=100; n=6; x=(0:m-1)/m; x=x'; a=randi(10,n,1); A=[];
        for j=1:n
          A = [A x.^(j-1)];
        end;
        yex=A*a; y=yex+(rand(m,1)-0.5);
octave] N=A'*A; b=A'*y; atilde=inv(N)*b;
        [Q,R]=qr(A); c=Q'*y; aQR=R\c;
        disp([a atilde aQR]);
    8.0000    8.0847    8.0847
    8.0000    7.1480    7.1480
    4.0000    4.2264    4.2264
    4.0000    8.7568    8.7568
   10.0000    2.7420    2.7420
    6.0000    9.0386    9.0386
octave]
```

Given data y, form A, find a, such that $\|e\| = \|Aa - y\|$ is minimized

MODEL REDUCTION

1. Projection of mappings

The least-squares problem

$$\min_{\boldsymbol{x}\in\mathbb{R}^n} \| \boldsymbol{y} - \boldsymbol{A}\boldsymbol{x} \| \tag{4.1}$$

focuses on a simpler representation of a data vector $\boldsymbol{y}\in\mathbb{R}^m$ as a linear combination of column vectors of $\boldsymbol{A}\in\mathbb{R}^{m\times n}$. Consider some phenomenon modeled as a function between vector spaces $\boldsymbol{f}: X \longrightarrow Y$, such that for input parameters $\boldsymbol{x}\in X$, the state of the system is $\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{x})$. For most models $\boldsymbol{f}$ is differentiable, a transcription of the condition that the system should not exhibit jumps in behavior when changing the input parameters. Then by appropriate choice of units and origin, a linearized model

$$\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}, \boldsymbol{A}\in\mathbb{R}^{m\times n},$$

is obtained if $\boldsymbol{y}\in C(\boldsymbol{A})$, expressed as (1) if $\boldsymbol{y}\notin C(\boldsymbol{A})$.

A simpler description is often sought, typically based on recognition that the inputs and outputs of the model can themselves be obtained as linear combinations $\boldsymbol{x} = \boldsymbol{B}\boldsymbol{u}$, $\boldsymbol{y} = \boldsymbol{C}\boldsymbol{v}$, involving a smaller set of parameters $\boldsymbol{u}\in\mathbb{R}^q$, $\boldsymbol{v}\in\mathbb{R}^p$, $p < m$, $q < n$. The column spaces of the matrices $\boldsymbol{B}\in\mathbb{R}^{n\times q}$, $\boldsymbol{C}\in\mathbb{R}^{m\times p}$ are vector subspaces of the original set of inputs and outputs, $C(\boldsymbol{B})\leq\mathbb{R}^n$, $C(\boldsymbol{C})\leq\mathbb{R}^m$. The sets of column vectors of $\boldsymbol{B}, \boldsymbol{C}$ each form a *reduced basis* for the system inputs and outputs if they are chosed to be of full rank. The reduced bases are assumed to have been orthonormalized through the Gram-Schmidt procedure such that $\boldsymbol{B}^T\boldsymbol{B} = \boldsymbol{I}_q$, and $\boldsymbol{C}^T\boldsymbol{C} = \boldsymbol{I}_p$. Expressing the model inputs and outputs in terms of the reduced basis leads to

$$\boldsymbol{C}\boldsymbol{v} = \boldsymbol{A}\boldsymbol{B}\boldsymbol{u} \Longrightarrow \boldsymbol{v} = \boldsymbol{C}^T\boldsymbol{A}\boldsymbol{B}\boldsymbol{u} \Longrightarrow \boldsymbol{v} = \boldsymbol{R}\boldsymbol{u}.$$

The matrix $\boldsymbol{R} = \boldsymbol{C}^T\boldsymbol{A}\boldsymbol{B}$ is called the *reduced system matrix* and is associated with a mapping $\boldsymbol{g}: U \longrightarrow V$, that is a restriction to the U, V vector subspaces of the mapping $\boldsymbol{f}$. When $\boldsymbol{f}$ is an endomorphism, $\boldsymbol{f}: X \longrightarrow X$, $m = n$, the same reduced basis is used for both inputs and outputs, $\boldsymbol{x} = \boldsymbol{B}\boldsymbol{u}$, $\boldsymbol{y} = \boldsymbol{B}\boldsymbol{v}$, and the reduced system is

$$\boldsymbol{v} = \boldsymbol{R}\boldsymbol{u}, \boldsymbol{R} = \boldsymbol{B}^T\boldsymbol{A}\boldsymbol{B}.$$

Since $\boldsymbol{B}$ is assumed to be orthogonal, the projector onto $C(\boldsymbol{B})$ is $\boldsymbol{P}_{\boldsymbol{B}} = \boldsymbol{B}\boldsymbol{B}^T$. Applying the projector on the inital model

$$\boldsymbol{P}_{\boldsymbol{B}}\boldsymbol{y} = \boldsymbol{P}_{\boldsymbol{B}}\boldsymbol{A}\boldsymbol{x}$$

leads to $\boldsymbol{B}\boldsymbol{B}^T\boldsymbol{y} = \boldsymbol{B}\boldsymbol{B}^T\boldsymbol{A}\boldsymbol{x}$, and since $\boldsymbol{v} = \boldsymbol{B}^T\boldsymbol{y}$ the relation $\boldsymbol{B}\boldsymbol{v} = \boldsymbol{B}\boldsymbol{B}^T\boldsymbol{A}\boldsymbol{B}\boldsymbol{u}$ is obtained, and conveniently grouped as

$$\boldsymbol{B}\boldsymbol{v} = \boldsymbol{B}\,(\boldsymbol{B}^T\boldsymbol{A}\boldsymbol{B})\,\boldsymbol{u} \Longrightarrow \boldsymbol{B}\boldsymbol{v} = \boldsymbol{B}(\boldsymbol{R}\boldsymbol{u}),$$

again leading to the reduced model $\boldsymbol{v} = \boldsymbol{B}\boldsymbol{u}$. The above calculation highlights that the reduced model is a projection of the full model $\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}$ on $C(\boldsymbol{B})$.

2. Reduced bases

2.1. Correlation matrices

Correlation coefficient. Consider two functions $x_1, x_2 : \mathbb{R} \longrightarrow \mathbb{R}$, that represent data streams in time of inputs $x_1(t)$ and outputs $x_2(t)$ of some system. A basic question arising in modeling and data science is whether the inputs and outputs are themselves in a functional relationship. This usually is a consequence of incomplete knowledge of the system, such that while x_1, x_2 might be assumed to be the most relevant input, output quantities, this is not yet fully established. A typical approach is to then carry out repeated measurements leading to a data set $D = \{(x_1(t_i), x_2(t_i)) \mid i = 1, \ldots, N\}$, thus defining a relation. Let $\boldsymbol{x}_1, \boldsymbol{x}_2 \in \mathbb{R}^N$ denote vectors containing the input and output values. The *mean values* μ_1, μ_2 of the input and output are estimated by the statistics

$$\mu_1 \cong \bar{x}_1 = \frac{1}{N}\sum_{i=1}^{N} x_1(t_i) = E[x_1], \mu_2 \cong \bar{x}_2 = \frac{1}{N}\sum_{i=1}^{N} x_2(t_i) = E[x_2],$$

where E is the expectation seen to be a linear mapping, $E : \mathbb{R}^N \longrightarrow \mathbb{R}$ whose associated matrix is

$$\boldsymbol{E} = \frac{1}{N}[\ 1\ \ 1\ \ \ldots\ \ 1\ ],$$

and the means are also obtained by matrix vector multiplication (linear combination),

$$\bar{x}_1 = \boldsymbol{E}\boldsymbol{x}_1,\ \bar{x}_2 = \boldsymbol{E}\boldsymbol{x}_2.$$

Deviation from the mean is measured by the *standard deviation* defined for x_1, x_2 by

$$\sigma_1 = \sqrt{E[(x_1 - \mu_1)^2]},\ \sigma_2 = \sqrt{E[(x_2 - \mu_2)^2]}.$$

Note that the standard deviations are no longer linear mappings of the data.

Assume that the origin is chosen such that $\bar{x}_1 = \bar{x}_2 = 0$. One tool to estalish whether the relation D is also a function is to compute the *correlation coefficient*

$$\rho(x_1, x_2) = \frac{E[x_1 x_2]}{\sigma_1\,\sigma_2} = \frac{E[x_1 x_2]}{\sqrt{E[x_1^2]\,E[x_2^2]}},$$

that can be expressed in terms of a scalar product and 2-norm as

$$\rho(x_1, x_2) = \frac{\boldsymbol{x}_1^T\boldsymbol{x}_2}{\|\boldsymbol{x}_1\|\ \|\boldsymbol{x}_2\|}.$$

Squaring each side of the norm property $\|\boldsymbol{x}_1+\boldsymbol{x}_2\| \leq \|\boldsymbol{x}_1\| + \|\boldsymbol{x}_2\|$, leads to

$$(\boldsymbol{x}_1+\boldsymbol{x}_2)^T(\boldsymbol{x}_1+\boldsymbol{x}_2) \leq \boldsymbol{x}_1^T\boldsymbol{x}_1 + \boldsymbol{x}_2^T\boldsymbol{x}_2 + 2\,\|\boldsymbol{x}_1\|\,\|\boldsymbol{x}_2\| \Longrightarrow \boldsymbol{x}_1^T\boldsymbol{x}_2 \leq \|\boldsymbol{x}_1\|\,\|\boldsymbol{x}_2\|,$$

known as the Cauchy-Schwarz inequality, which implies $-1 \leq \rho(x_1,x_2) \leq 1$. Depending on the value of ρ, the variables $x_1(t), x_2(t)$ are said to be:

1. *uncorrelated*, if $\rho = 0$;
2. *correlated*, if $\rho = 1$;
3. *anti-correlated*, if $\rho = -1$.

The numerator of the correlation coefficient is known as the covariance of x_1, x_2

$$\text{cov}(x_1,x_2) = E[x_1x_2].$$

The correlation coefficient can be interpreted as a normalization of the covariance, and the relation

$$\text{cov}(x_1,x_2) = \boldsymbol{x}_1^T\boldsymbol{x}_2 = \rho(x_1,x_2)\,\|\boldsymbol{x}_1\|\,\|\boldsymbol{x}_2\|,$$

is the two-variable version of a more general relationship encountered when the system inputs and outputs become vectors.

Patterns in data. Consider now a related problem, whether the input and output parameters $\boldsymbol{x} \in \mathbb{R}^n$, $\boldsymbol{y} \in \mathbb{R}^m$ thought to characterize a system are actually well chosen, or whether they are redundant in the sense that a more insightful description is furnished by $\boldsymbol{u} \in \mathbb{R}^q$, $\boldsymbol{v} \in \mathbb{R}^p$ with fewer components $p < m, q < n$. Applying the same ideas as in the correlation coefficient, a sequence of N measurements is made leading to data sets

$$\boldsymbol{X} = \begin{bmatrix} \boldsymbol{x}_1 & \boldsymbol{x}_2 & \dots & \boldsymbol{x}_n \end{bmatrix} \in \mathbb{R}^{N\times n}, \boldsymbol{Y} = \begin{bmatrix} \boldsymbol{y}_1 & \boldsymbol{y}_2 & \dots & \boldsymbol{y}_n \end{bmatrix} \in \mathbb{R}^{N\times m}.$$

Again, by appropriate choice of the origin the means of the above measurements is assumed to be zero

$$E[\boldsymbol{x}] = \boldsymbol{0}, E[\boldsymbol{y}] = \boldsymbol{0}.$$

Covariance matrices can be constructed by

$$\boldsymbol{C_X} = \boldsymbol{X}^T\boldsymbol{X} = \begin{bmatrix} \boldsymbol{x}_1^T \\ \boldsymbol{x}_2^T \\ \vdots \\ \boldsymbol{x}_n^T \end{bmatrix} \begin{bmatrix} \boldsymbol{x}_1 & \boldsymbol{x}_2 & \dots & \boldsymbol{x}_n \end{bmatrix} = \begin{bmatrix} \boldsymbol{x}_1^T\boldsymbol{x}_1 & \boldsymbol{x}_1^T\boldsymbol{x}_2 & \dots & \boldsymbol{x}_1^T\boldsymbol{x}_n \\ \boldsymbol{x}_2^T\boldsymbol{x}_1 & \boldsymbol{x}_2^T\boldsymbol{x}_2 & \dots & \boldsymbol{x}_2^T\boldsymbol{x}_n \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{x}_n^T\boldsymbol{x}_1 & \boldsymbol{x}_n^T\boldsymbol{x}_2 & \dots & \boldsymbol{x}_n^T\boldsymbol{x}_n \end{bmatrix} \in \mathbb{R}^{n\times n}.$$

Consider now the SVDs of $C_{\boldsymbol{X}} = \boldsymbol{N}\boldsymbol{\Lambda}\boldsymbol{N}^T$, $\boldsymbol{X} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{S}^T$, and from

$$\boldsymbol{C_X} = \boldsymbol{X}^T\boldsymbol{X} = (\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{S}^T)^T\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{S}^T = \boldsymbol{S}\boldsymbol{\Sigma}^T\boldsymbol{U}^T\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{S}^T = \boldsymbol{S}\boldsymbol{\Sigma}^T\boldsymbol{\Sigma}\boldsymbol{S}^T = \boldsymbol{N}\boldsymbol{\Lambda}\boldsymbol{N}^T,$$

identify $\boldsymbol{N} = \boldsymbol{S}$, and $\boldsymbol{\Lambda} = \boldsymbol{\Sigma}^T\boldsymbol{\Sigma}$.

Recall that the SVD returns an order set of singular values $\sigma_1 \geqslant \sigma_2 \geqslant \cdots \geqslant$, and associated singular vectors. In many applications the singular values decrease quickly, often exponentially fast. Taking the first q singular modes then gives a basis set suitable for mode reduction

$$\boldsymbol{x} = \boldsymbol{S}_q \, \boldsymbol{u} = \begin{bmatrix} \boldsymbol{s}_1 & \boldsymbol{s}_2 & \dots & \boldsymbol{s}_q \end{bmatrix} \boldsymbol{u}.$$

CHAPTER 5

CHANGE OF BASIS

DATA TRANSFORMATION

1. Gaussian elimination and row echelon reduction

Suppose now that $A\,x = b$ admits a unique solution. How to find it? We are especially interested in constructing a general procedure, that will work no matter what the size of A might be. This means we seek an *algorithm* that precisely specifies the steps that lead to the solution, and that we can program a computing device to carry out automatically. One such algorithm is *Gaussian elimination.*

Consider the system

$$\begin{cases} x_1 + 2\,x_2 - x_3 &= 2 \\ 2\,x_1 - x_2 + x_3 &= 2 \\ 3\,x_1 - x_2 - x_3 &= 1 \end{cases}$$

The idea is to combine equations such that we have one fewer unknown in each equation. Ask: with what number should the first equation be multiplied in order to eliminate x_1 from sum of equation 1 and equation 2? This number is called a Gaussian multiplier, and is in this case -2. Repeat the question for eliminating x_1 from third equation, with multiplier -3.

$$\begin{cases} x_1 + 2\,x_2 - x_3 &= 2 \\ 2\,x_1 - x_2 + x_3 &= 2 \\ 3\,x_1 - x_2 - x_3 &= 1 \end{cases} \Longrightarrow \begin{cases} x_1 + 2\,x_2 - x_3 &= 2 \\ -5\,x_2 + 3\,x_3 &= -2 \\ -7\,x_2 + 2\,x_3 &= -5 \end{cases}$$

Now, ask: with what number should the second equation be multiplied to eliminate x_2 from sum of second and third equations. The multiplier is in this case $-7/5$.

$$\begin{cases} x_1 + 2\,x_2 - x_3 &= 2 \\ -5\,x_2 + 3\,x_3 &= -2 \\ -7\,x_2 + 2\,x_3 &= -5 \end{cases} \Longrightarrow \begin{cases} x_1 + 2\,x_2 - x_3 &= 2 \\ -5\,x_2 + 3\,x_3 &= -2 \\ -\dfrac{11}{5}\,x_3 &= -\dfrac{11}{5} \end{cases}$$

Starting from the last equation we can now find $x_3 = 1$, replace in the second to obtain $-5\,x_2 = -5$, hence $x_2 = 1$, and finally replace in the first equation to obtain $x_1 = 1$.

The above operations only involve coefficients. A more compact notation is therefore to work with what is known as the "bordered matrix"

$$\begin{pmatrix} 1 & 2 & -1 & 2 \\ 2 & -1 & 1 & 2 \\ 3 & -1 & -1 & 1 \end{pmatrix} \sim \begin{pmatrix} 1 & 2 & -1 & 2 \\ 0 & -5 & 3 & -2 \\ 0 & -7 & 2 & -5 \end{pmatrix} \sim \begin{pmatrix} 1 & 2 & -1 & 2 \\ 0 & -5 & 3 & -2 \\ 0 & 0 & -\dfrac{11}{5} & -\dfrac{11}{5} \end{pmatrix}$$

Once the above *triangular* form has been obtain, the solution is found by back substitution, in which we seek to form the identity matrix in the first 3 columns, and the solution is obtained in the last column.

$$\begin{pmatrix} 1 & 2 & -1 & 2 \\ 0 & -5 & 3 & -2 \\ 0 & 0 & -\frac{11}{5} & -\frac{11}{5} \end{pmatrix} \sim \begin{pmatrix} 1 & 2 & -1 & 2 \\ 0 & -5 & 3 & -2 \\ 0 & 0 & 1 & 1 \end{pmatrix} \sim \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}$$

2. LU-factorization

- We have introduced Gaussian elimination as a procedure to solve the linear system $A\,x = b$ ("find coordinates of vector b in terms of column vectors of matrix A"), $x, b \in \mathbb{R}^m, A \in \mathbb{R}^{m \times m}$
- We now reinterpret Gaussian elimination as a sequence of matrix multiplications applied to A to obtain a simpler, upper triangular form.

2.1. Example for $m = 3$

Consider the system $A\,x = b$

$$\begin{cases} x_1 + 2\,x_2 - x_3 &= 2 \\ 2\,x_1 - x_2 + x_3 &= 2 \\ 3\,x_1 - x_2 - x_3 &= 1 \end{cases}$$

with

$$A = \begin{pmatrix} 1 & 2 & -1 \\ 2 & -1 & 1 \\ 3 & -1 & -1 \end{pmatrix}, b = \begin{pmatrix} 2 \\ 2 \\ 1 \end{pmatrix}$$

We ask if there is a matrix L_1 that could be multiplied with A to produce a result $L_1 A$ with zeros under the main diagonal in the first column. First, gain insight by considering multiplication by the identity matrix, which leaves A unchanged

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 2 & -1 \\ 2 & -1 & 1 \\ 3 & -1 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 2 & -1 \\ 2 & -1 & 1 \\ 3 & -1 & -1 \end{pmatrix}$$

In the first stage of Gaussian multiplication, the first line remains unchanged, so we deduce that L_1 should have the same first line as the identity matrix

$$L_1 = \begin{pmatrix} 1 & 0 & 0 \\ ? & ? & ? \\ ? & ? & ? \end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 & 0 \\ ? & ? & ? \\ ? & ? & ? \end{pmatrix} \begin{pmatrix} 1 & 2 & -1 \\ 2 & -1 & 1 \\ 3 & -1 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 2 & -1 \\ 0 & -5 & 3 \\ 0 & -7 & 2 \end{pmatrix}$$

Next, recall the way Gaussian multipliers were determined: find number to multiply first line so that added to second, third lines a zero is obtained. This leads to the form

$$L_1 = \begin{pmatrix} 1 & 0 & 0 \\ ? & 1 & 0 \\ ? & 0 & 1 \end{pmatrix}$$

Finally, identify the missing entries with the Gaussian multipliers to determine

$$L_1 = \begin{pmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ -3 & 0 & 1 \end{pmatrix}$$

Verify by carrying out the matrix multiplication

$$L_1 A = \begin{pmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ -3 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 2 & -1 \\ 2 & -1 & 1 \\ 3 & -1 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 2 & -1 \\ 0 & -5 & 3 \\ 0 & -7 & 2 \end{pmatrix}$$

Repeat the above reasoning to come up with a second matrix L_2 that forms a zero under the main diagonal in the second column

$$L_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -7/5 & 1 \end{pmatrix}$$

$$L_2 L_1 A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -7/5 & 1 \end{pmatrix} \begin{pmatrix} 1 & 2 & -1 \\ 0 & -5 & 3 \\ 0 & -7 & 2 \end{pmatrix} = \begin{pmatrix} 1 & 2 & -1 \\ 0 & -5 & 3 \\ 0 & 0 & -11/5 \end{pmatrix} = U$$

We have obtained a matrix with zero entries under the main diagonal (an upper triangular matrix) by a sequence of matrix multiplications.

2.2. General m case

From the above, we assume that we can form a sequence of multiplier matrices such that the result is an upper triangular matrix U

$$L_{m-1} \ldots L_2 L_1 A = U$$

- Recall the basic operation in row echelon reduction: constructing a linear combination of rows to form zeros beneath the main diagonal, e.g.

$$\boldsymbol{A} = \begin{pmatrix} a_{11} & a_{12} & \ldots & a_{1m} \\ a_{21} & a_{22} & \ldots & a_{2m} \\ a_{31} & a_{32} & \ldots & a_{3m} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \ldots & a_{mm} \end{pmatrix} \sim \begin{pmatrix} a_{11} & a_{12} & \ldots & a_{1m} \\ 0 & a_{22} - \frac{a_{21}}{a_{11}} a_{12} & \ldots & a_{2m} - \frac{a_{21}}{a_{11}} a_{1m} \\ 0 & a_{32} - \frac{a_{31}}{a_{11}} a_{12} & \ldots & a_{3m} - \frac{a_{31}}{a_{11}} a_{1m} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & a_{m2} - \frac{a_{m1}}{a_{11}} a_{12} & \ldots & a_{mm} - \frac{a_{m1}}{a_{11}} a_{1m} \end{pmatrix}$$

- This can be stated as a matrix multiplication operation, with $l_{i1} = a_{i1}/a_{11}$

$$\begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ -l_{21} & 1 & 0 & \dots & 0 \\ -l_{31} & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -l_{m1} & 0 & 0 & \dots & 1 \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1m} \\ a_{21} & a_{22} & \dots & a_{2m} \\ a_{31} & a_{32} & \dots & a_{3m} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mm} \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1m} \\ 0 & a_{22} - l_{21}a_{12} & \dots & a_{2m} - l_{21}a_{1m} \\ 0 & a_{32} - l_{31}a_{12} & \dots & a_{3m} - l_{31}a_{1m} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & a_{m2} - l_{m1}a_{12} & \dots & a_{mm} - l_{m1}a_{1m} \end{pmatrix}$$

DEFINITION. *The matrix*

$$\boldsymbol{L}_k = \begin{pmatrix} 1 & \dots & 0 & \dots & 1 \\ 0 & \ddots & 0 & \dots & 0 \\ 0 & \dots & 1 & \dots & 0 \\ 0 & \dots & -l_{k+1,k} & \dots & 0 \\ 0 & \dots & -l_{k+2,k} & \dots & 0 \\ \vdots & \dots & \vdots & \ddots & \vdots \\ 0 & \dots & -l_{m,k} & \dots & 1 \end{pmatrix}$$

with $l_{i,k} = a_{i,k}^{(k)}/a_{k,k}^{(k)}$, and $\boldsymbol{A}^{(k)} = (a_{i,j}^{(k)})$ the matrix obtained after step k of row echelon reduction (or, equivalently, Gaussian elimination) is called a Gaussian multiplier matrix.

- For $\boldsymbol{A} \in \mathbb{R}^{m \times m}$ nonsingular, the successive steps in row echelon reduction (or Gaussian elimination) correspond to successive multiplications on the left by Gaussian multiplier matrices

$$\boldsymbol{L}_{m-1}\boldsymbol{L}_{m-2}\dots\boldsymbol{L}_2\boldsymbol{L}_1\boldsymbol{A} = \boldsymbol{U}$$

- The inverse of a Gaussian multiplier is

$$\boldsymbol{L}_k^{-1} = \begin{pmatrix} 1 & \dots & 0 & \dots & 1 \\ 0 & \ddots & 0 & \dots & 0 \\ 0 & \dots & 1 & \dots & 0 \\ 0 & \dots & l_{k+1,k} & \dots & 0 \\ 0 & \dots & l_{k+2,k} & \dots & 0 \\ \vdots & \dots & \vdots & \ddots & \vdots \\ 0 & \dots & l_{m,k} & \dots & 1 \end{pmatrix} = \boldsymbol{I} - (\boldsymbol{L}_k - \boldsymbol{I})$$

- From $(\boldsymbol{L}_{m-1}\boldsymbol{L}_{m-2}\dots\boldsymbol{L}_2\boldsymbol{L}_1)\boldsymbol{A} = \boldsymbol{U}$ obtain

$$\boldsymbol{A} = (\boldsymbol{L}_{m-1}\boldsymbol{L}_{m-2}\dots\boldsymbol{L}_2\boldsymbol{L}_1)^{-1}\boldsymbol{U} = \boldsymbol{L}_1^{-1}\boldsymbol{L}_2^{-1}\cdot\ldots\cdot\boldsymbol{L}_{m-1}^{-1}\boldsymbol{U} = \boldsymbol{L}\,\boldsymbol{U}$$

- Due to the simple form of $\boldsymbol{L}_k^{-1}$ the matrix $\boldsymbol{L}$ is easily obtained as

$$\boldsymbol{L} = \begin{pmatrix} 1 & 0 & 0 & \dots & 0 & 0 \\ l_{2,1} & 1 & 0 & \dots & 0 & 0 \\ l_{3,1} & l_{3,2} & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ l_{m-1,1} & l_{m-1,2} & l_{m-1,3} & \dots & 1 & 0 \\ l_{m,1} & l_{m,2} & l_{m,3} & \dots & l_{m,m-1} & 1 \end{pmatrix}$$

We will show that this indeed possible if $A\,x = b$ admits a unique solution. Furthermore, the product of lower triangular matrices is lower triangular, and the inverse of a lower triangular matrix is lower triangular (same applies for upper triangular matrices). Introduce the notation

$$L^{-1} = L_{m-1} \ldots L_2 L_1$$

and obtain

$$L^{-1} A = U$$

or

$$A = L\,U$$

The above result permits a basic insight into Gaussian elimination: the procedure depends on "factoring" the matrix A into two "simpler" matrices L, U. The idea of representing a matrix as a product of simpler matrices is fundamental to linear algebra, and we will come across it repeatedly.

For now, the factorization allows us to devise the following general approach to solving $A\,x = b$

1. Find the factorization $L\,U = A$

2. Insert the factorization into $A\,x = b$ to obtain $(L\,U)\,x = L\,(U\,x) = L\,y = b$, where the notation $y = U\,x$ has been introduced. The system

   $$L\,y = b$$

   is easy to solve by forward substitution to find y for given b

3. Finally find x by backward substitution solution of

   $$U\,x = y$$

Algorithm Gauss elimination without pivoting

for $s = 1$ to $m - 1$
  for $i = s + 1$ to m
    $t = -a_{is} / a_{ss}$
    for $j = s + 1$ to m
      $a_{ij} = a_{ij} + t \cdot a_{sj}$
    $b_i = b_i + t \cdot b_s$

for $s = m$ downto 1
  $x_s = b_s / a_{ss}$
  for $i = 1$ to $s - 1$
    $b_i = b_i - a_{is} \cdot x_s$

return x

Algorithm Gauss elimination with partial pivoting

$p = 1{:}m$ (initialize row permutation vector)
for $s = 1$ to $m-1$
  piv = abs($a_{p(s),s}$)
  for $i = s+1$ to m
    mag = abs($a_{p(i),s}$)
    if mag > piv then
      piv = mag; $k = p(s); p(s) = p(i); p(i) = k$
    if piv < ϵ then break("Singular matrix")
    $t = -a_{p(i)s} / a_{p(s)s}$
    for $j = s+1$ to m
      $a_{p(i)j} = a_{p(i)j} + t \cdot a_{p(s)j}$
    $b_{p(i)} = b_{p(i)} + t \cdot b_{p(s)}$

for $s = m$ downto 1
  $x_s = b_{p(s)} / a_{p(s)s}$
  for $i = 1$ to $s-1$
    $b_{p(i)} = b_{p(i)} - a_{p(i)s} \cdot x_s$

return x

Given $\boldsymbol{A} \in \mathbb{R}^{m \times n}$

Singular value decomposition	Gram-Schmidt	Lower-upper
Transformation of coordinates	$\boldsymbol{Ax} = \boldsymbol{b}$	
$\boldsymbol{U\Sigma V^T} = \boldsymbol{A}$	$\boldsymbol{QR} = \boldsymbol{A}$	$\boldsymbol{LU} = \boldsymbol{A}$
$(\boldsymbol{U\Sigma V^T})\boldsymbol{x} = \boldsymbol{b} \Longrightarrow \boldsymbol{Uy} = \boldsymbol{b} \Longrightarrow \boldsymbol{y} = \boldsymbol{U^T b}$	$(\boldsymbol{QR})\boldsymbol{x} = \boldsymbol{b} \Longrightarrow \boldsymbol{Qy} = \boldsymbol{b},\ \boldsymbol{y} = \boldsymbol{Q^T b}$	$(\boldsymbol{LU})\boldsymbol{x} = \boldsymbol{b} \Longrightarrow \boldsymbol{Ly} = \boldsymbol{b}$ (forward sub to find) $\mathbf{y}$
$\boldsymbol{\Sigma z} = \boldsymbol{y} \Longrightarrow \boldsymbol{z} = \boldsymbol{\Sigma^+ y}$	$\boldsymbol{Rx} = \boldsymbol{y}$ (back sub to find $\boldsymbol{x}$)	$\boldsymbol{Ux} = \boldsymbol{y}$ (back sub to find $\boldsymbol{x}$)
$\boldsymbol{V^T x} = \boldsymbol{z} \Longrightarrow \boldsymbol{x} = \boldsymbol{Vz}$		

3. Inverse matrix

By analogy to the simple scalar equation $a\,x = b$ with solution $x = a^{-1}\,b$ when $a \neq 0$, we are interested in writing the solution to a linear system $A\,x = b$ as $x = A^{-1}\,b$ for $A \in \mathbb{R}^{m \times m}$, $x \in \mathbb{R}^m$. Recall that solving $A\,x = b = I\,b$ corresponds to expressing the vector b as a linear combination of the columns of A. This can only be done if the columns of A form a basis for $\mathbb{R}^m$, in which case we say that A is *non-singular*.

DEFINITION 5.1. *For matrix $A \in \mathbb{R}^{m \times m}$ non-singular the inverse matrix is denoted by A^{-1} and satisfies the properties*

$$A\,A^{-1} = A^{-1}\,A = I$$

3.1. Gauss-Jordan algorithm

Computation of the inverse A^{-1} can be carried out by repeated use of Gauss elimination. Denote the inverse by $B = A^{-1}$ for a moment and consider the inverse matrix property $A\ B = I$. Introducing the column notation for B, I leads to

$$A(\ B_1\ \ ...\ \ B_m\ ) = (\ e_1\ \ ...\ \ e_m\ )$$

and identification of each column in the equality states

$$A\,B_k = e_k, k = 1, 2, .., m$$

with e_k the column unit vector with zero components everywhere except for a 1 in row k. To find the inverse we need to simultaneously solve the m linear systems given above.

Gauss-Jordan algorithm example. Consider

$$A = \begin{pmatrix} 1 & 2 & 3 \\ -1 & 3 & 1 \\ 2 & -1 & -2 \end{pmatrix}$$

To find the inverse we solve the systems $A\ B_1 = e_1, A\ B_2 = e_2, A\ B_3 = e_3$. This can be done simultaneously by working with the matrix A bordered by I

$$(A \mid I) = \begin{pmatrix} 1 & 1 & 0 & 1 & 0 & 0 \\ -1 & 1 & 1 & 0 & 1 & 0 \\ 2 & 4 & -2 & 0 & 0 & 1 \end{pmatrix}$$

Carry out now operations involving linear row combinations and permutations to bring the left side to I

$$\begin{pmatrix} 1 & 1 & 0 & 1 & 0 & 0 \\ -1 & 1 & 1 & 0 & 1 & 0 \\ 2 & 4 & -2 & 0 & 0 & 1 \end{pmatrix} \sim \begin{pmatrix} 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 2 & 1 & 1 & 1 & 0 \\ 0 & 2 & -2 & -2 & 0 & 1 \end{pmatrix} \sim \begin{pmatrix} 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 2 & 1 & 1 & 1 & 0 \\ 0 & 0 & -3 & -3 & -1 & 1 \end{pmatrix} \sim$$

$$\sim \begin{pmatrix} 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 2 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & \frac{1}{3} & -\frac{1}{3} \end{pmatrix} \sim \begin{pmatrix} 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 2 & 0 & 0 & \frac{2}{3} & \frac{1}{3} \\ 0 & 0 & 1 & 1 & \frac{1}{3} & -\frac{1}{3} \end{pmatrix} \sim \begin{pmatrix} 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & \frac{1}{3} & \frac{1}{6} \\ 0 & 0 & 1 & 1 & \frac{1}{3} & -\frac{1}{3} \end{pmatrix} \sim$$

$$\begin{pmatrix} 1 & 0 & 0 & 1 & -\frac{1}{3} & -\frac{1}{6} \\ 0 & 1 & 0 & 0 & \frac{1}{3} & \frac{1}{6} \\ 0 & 0 & 1 & 1 & \frac{1}{3} & -\frac{1}{3} \end{pmatrix}$$

to obtain

$$A^{-1} = \begin{pmatrix} 1 & -\frac{1}{3} & -\frac{1}{6} \\ 0 & \frac{1}{3} & \frac{1}{6} \\ 1 & \frac{1}{3} & -\frac{1}{3} \end{pmatrix}$$

4. Determinants

- $\boldsymbol{A} \in \mathbb{R}^{m \times m}$ a square matrix, $\det(\boldsymbol{A}) \in \mathbb{R}$ is the oriented volume enclosed by the column vectors of $\boldsymbol{A}$ (a parallelipiped)
- Geometric interpretation of determinants
- Determinant calculation rules
- Algebraic definition of a determinant

DEFINITION. *The determinant of a square matrix* $\boldsymbol{A} = (\, \boldsymbol{a}_1 \ \dots \ \boldsymbol{a}_m \,) \in \mathbb{R}^{m \times m}$ *is a real number*

$$\det(A) = \begin{vmatrix} a_{11} & a_{12} & \dots & a_{1m} \\ a_{21} & a_{22} & \dots & a_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mm} \end{vmatrix} \in \mathbb{R}$$

giving the (oriented) volume of the parallelepiped spanned by matrix column vectors.

- $m = 2$

$$\boldsymbol{A} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, \det(\boldsymbol{A}) = \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix}$$

- $m = 3$

$$\boldsymbol{A} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}, \det(\boldsymbol{A}) = \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix}$$

- Computation of a determinant with $m = 2$

$$\begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = a_{11}a_{22} - a_{12}a_{21}$$

- Computation of a determinant with $m = 3$

$$\begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} = a_{11}a_{22}a_{33} + a_{21}a_{32}a_{13} + a_{31}a_{12}a_{23} - a_{13}a_{22}a_{31} - a_{23}a_{32}a_{11} - a_{33}a_{12}a_{21}$$

- Where do these determinant computation rules come from? Two viewpoints
  - *Geometric viewpoint*: determinants express parallelepiped volumes
  - *Algebraic viewpoint*: determinants are computed from all possible products that can be formed from choosing a factor from each row and each column
- $m = 2$

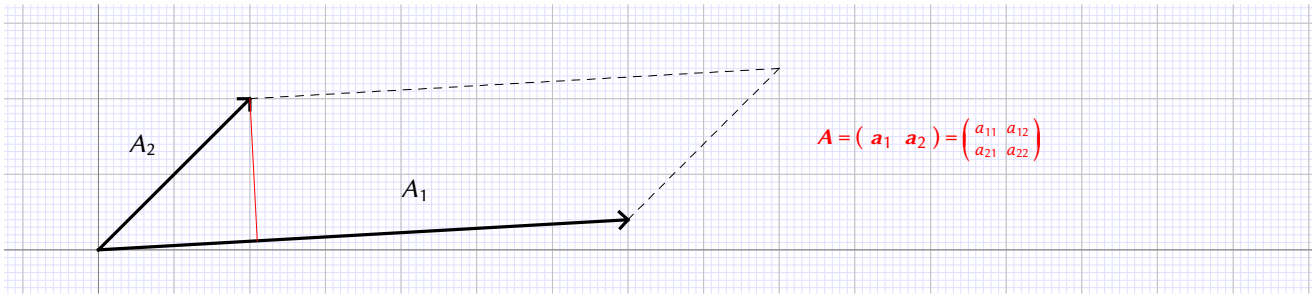


Figure 5.1.

- In two dimensions a ``parallelepiped'' becomes a parallelogram with area given as

$$(\text{Area}) = (\text{Length of Base}) \times (\text{Length of Height})$$

- Take $\boldsymbol{a}_1$ as the base, with length $b = \|\boldsymbol{a}_1\|$. Vector $\boldsymbol{a}_1$ is at angle φ_1 to x_1-axis, $\boldsymbol{a}_2$ is at angle φ_2 to x_2-axis, and the angle between $\boldsymbol{a}_1$, $\boldsymbol{a}_2$ is $\theta = \varphi_2 - \varphi_1$. The height has length

$$h = \|\boldsymbol{a}_2\| \sin\theta = \|\boldsymbol{a}_2\| \sin(\varphi_2 - \varphi_1) = \|\boldsymbol{a}_2\| (\sin\varphi_2 \cos\varphi_1 - \sin\varphi_1 \cos\varphi_2)$$

- Use $\cos\varphi_1 = a_{11}/\|\boldsymbol{a}_1\|$, $\sin\varphi_1 = a_{12}/\|\boldsymbol{a}_1\|$, $\cos\varphi_2 = a_{21}/\|\boldsymbol{a}_2\|$, $\sin\varphi_2 = a_{22}/\|\boldsymbol{a}_2\|$

$$(\text{Area}) = \|\boldsymbol{a}_1\|\ \|\boldsymbol{a}_2\| (\sin\varphi_2 \cos\varphi_1 - \sin\varphi_1 \cos\varphi_2) = a_{11}a_{22} - a_{12}a_{21}$$

- The geometric interpretation of a determinant as an oriented volume is useful in establishing rules for calculation with determinants:
  - Determinant of matrix with repeated columns is zero (since two edges of the parallelepiped are identical). Example for $m = 3$

$$\Delta = \begin{vmatrix} a & a & u \\ b & b & v \\ c & c & w \end{vmatrix} = abw + bcu + cav - ubc - vca - wab = 0$$

This is more easily seen using the column notation

$$\Delta = \det(\ \boldsymbol{a}_1\ \ \boldsymbol{a}_1\ \ \boldsymbol{a}_3\ \ \ldots\ ) = 0$$

  - Determinant of matrix with linearly dependent columns is zero (since one edge lies in the 'hyperplane' formed by all the others)

- Separating sums in a column (similar for rows)

$$\det(\ \boldsymbol{a}_1+\boldsymbol{b}_1\ \ \boldsymbol{a}_2\ \ \dots\ \ \boldsymbol{a}_m\ )=\det(\ \boldsymbol{a}_1\ \ \boldsymbol{a}_2\ \ \dots\ \ \boldsymbol{a}_m\ )+\det(\ \boldsymbol{b}_1\ \ \boldsymbol{a}_2\ \ \dots\ \ \boldsymbol{a}_m\ )$$

  with $\boldsymbol{a}_i, \boldsymbol{b}_1 \in \mathbb{R}^m$

- Scalar product in a column (similar for rows)

$$\det(\ \alpha\boldsymbol{a}_1\ \ \boldsymbol{a}_2\ \ \dots\ \ \boldsymbol{a}_m\ )=\alpha\det(\ \boldsymbol{a}_1\ \ \boldsymbol{a}_2\ \ \dots\ \ \boldsymbol{a}_m\ )$$

  with $\alpha \in \mathbb{R}$

- Linear combinations of columns (similar for rows)

$$\det(\ \boldsymbol{a}_1\ \ \boldsymbol{a}_2\ \ \dots\ \ \boldsymbol{a}_m\ )=\det(\ \boldsymbol{a}_1\ \ \alpha\boldsymbol{a}_1+\boldsymbol{a}_2\ \ \dots\ \ \boldsymbol{a}_m\ )$$

  with $\alpha \in \mathbb{R}$.

- A determinant of size m can be expressed as a sum of determinants of size $m-1$ by expansion along a row or column

$$\begin{vmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1m} \\ a_{21} & a_{22} & a_{23} & \dots & a_{2m} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & a_{m3} & \dots & a_{mm} \end{vmatrix} = a_{11}\begin{vmatrix} a_{22} & a_{23} & \dots & a_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m2} & a_{m3} & \dots & a_{mm} \end{vmatrix} -$$
$$a_{12}\begin{vmatrix} a_{21} & a_{23} & \dots & a_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m3} & \dots & a_{mm} \end{vmatrix} +$$
$$a_{13}\begin{vmatrix} a_{21} & a_{22} & a_{24} & \dots & a_{2m} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & a_{m4} & \dots & a_{mm} \end{vmatrix} -$$
$$\dots$$
$$+(-1)^{m+1}a_{1m}\begin{vmatrix} a_{21} & a_{23} & \dots & a_{2,m-1} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m3} & \dots & a_{m,m-1} \end{vmatrix}$$

- The formal definition of a determinant

$$\det A=\sum_{\sigma\in\Sigma}\nu(\sigma)a_{1i_1}a_{2i_2}\dots a_{mi_m}$$

  requires $mm!$ operations, a number that rapidly increases with m

- A more economical determinant is to use row and column combinations to create zeros and then reduce the size of the determinant, an algorithm reminiscent of Gauss elimination for systems

Example:

$$\begin{vmatrix} 1 & 2 & 3 \\ -1 & 0 & 1 \\ -2 & -1 & 4 \end{vmatrix} = \begin{vmatrix} 1 & 2 & 3 \\ 0 & 2 & 4 \\ 0 & 3 & 10 \end{vmatrix} = \begin{vmatrix} 2 & 4 \\ 3 & 10 \end{vmatrix} = 20 - 12 = 8$$

The first equality comes from linear combinations of rows, i.e. row 1 is added to row 2, and row 1 multiplied by 2 is added to row 3. These linear combinations maintain the value of the determinant. The second equality comes from expansion along the first column

4.1. Cross product

- Consider $u, v \in \mathbb{R}^3$. We've introduced the idea of a scalar product

$$u \cdot v = u^T v = u_1 v_1 + u_2 v_2 + u_3 v_3$$

in which from two vectors one obtains a scalar

- We've also introduced the idea of an exterior product

$$u v^T = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} \begin{pmatrix} v_1 & v_2 & v_3 \end{pmatrix} = \begin{pmatrix} u_1 v_1 & u_1 v_2 & u_1 v_3 \\ u_2 v_1 & u_2 v_2 & u_2 v_3 \\ u_3 v_1 & u_3 v_2 & u_3 v_3 \end{pmatrix}$$

in which a matrix is obtained from two vectors

- Another product of two vectors is also useful, the cross product, most conveniently expressed in determinant-like form

$$u \times v = \begin{vmatrix} \boldsymbol{e}_1 & \boldsymbol{e}_2 & \boldsymbol{e}_3 \\ u_1 & u_2 & u_3 \\ v_1 & v_2 & v_3 \end{vmatrix} = (u_2 v_3 - v_2 u_3)\boldsymbol{e}_1 + (u_3 v_1 - v_3 u_1)\boldsymbol{e}_2 + (u_1 v_2 - v_1 u_2)\boldsymbol{e}_3$$

DATA EFFICIENCY

1. Krylov bases

In reduction of the model

$$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{y}, \boldsymbol{A} \in \mathbb{R}^{m \times n}, \mathbb{R}^n \xrightarrow{\boldsymbol{A}} \mathbb{R}^m$$

by restriction to a subspaces spanned by the orthogonal column vectors of $\boldsymbol{B}, \boldsymbol{C}$, $\boldsymbol{x} = \boldsymbol{B}\boldsymbol{u}$, $\boldsymbol{y} = \boldsymbol{C}\boldsymbol{v}$, the reduced model

$$\boldsymbol{v} = \boldsymbol{R}\boldsymbol{u}$$

is obtained with $\boldsymbol{R} = \boldsymbol{C}^T \boldsymbol{A} \boldsymbol{B}$, the reduced system matrix. The choice of the basis sets $\boldsymbol{B}, \boldsymbol{C}$ is not yet specified. One common choice is to use the singular value decomposition $\boldsymbol{A} = \boldsymbol{S} \boldsymbol{\Sigma} \boldsymbol{Q}^T$ and choose the dominant k singular vectors to span the subspaces,

$$\boldsymbol{B} = \boldsymbol{Q}_k, \boldsymbol{C} = \boldsymbol{S}_k.$$

This assumes that an SVD is available, and that ordering of vectors by the 2-norm is relevant to the problem. This is often the case in problems in which the matrix $\boldsymbol{A}$ somewhow expresses the energy of a system. For example in deformation of a structure a relationship between forces $\boldsymbol{f}$ and displacements $\boldsymbol{u}$ is approximated linearly by $\boldsymbol{f} = \boldsymbol{K}\boldsymbol{u}$, with the stiffness matrix $\boldsymbol{K}$ expressing the potential energy stored in the deformation.

However in many cases, the model might not express an energy so the 2-norm is not an appropriate functional, or even if it is the size of the problem might render the computation of the singular value decomposition impractical. In such situations alternative procedures to construct reduced bases must be devised.

Consider that the only information available about the problem are the matrix $\boldsymbol{A} \in \mathbb{R}^{m \times m}$ and a vector $\boldsymbol{y} \in \mathbb{R}^m$. From these two a sequence of vectors can be gather into what is known as a *Krylov matrix*

$$\boldsymbol{K}_n = \begin{bmatrix} \boldsymbol{y} & \boldsymbol{A}\boldsymbol{y} & \boldsymbol{A}^2\boldsymbol{y} & \dots & \boldsymbol{A}^{n-1}\boldsymbol{y} \end{bmatrix}.$$

The Krylov matrix $\boldsymbol{K}_n$ is generally not orthogonal, but an orthogonal basis can readily be extracted through the QR factorization

$$\boldsymbol{Q}_n \boldsymbol{R} = \boldsymbol{K}_n.$$

The basis $\boldsymbol{Q}_n$ can then be adopted, both for the domain and the codomain

$$\boldsymbol{B} = \boldsymbol{C} = \boldsymbol{Q}_n.$$

2. Greedy approximation

The Krylov procedure has the virtue of simplicity, but does not have the desirable property of the SVD of ordering of the singular vectors. Suppose that the system matrix $\boldsymbol{A} \in \mathbb{R}^{m \times m}$ is applied to k vectors $\boldsymbol{x}_1, \dots, \boldsymbol{x}_k$, leading to formation of the vector set $S = \{\boldsymbol{A}\boldsymbol{x}_1, \dots, \boldsymbol{A}\boldsymbol{x}_k\}$. Denote by $\boldsymbol{B}$ the first n members of the set ordered in some arbitrary norm

$$\boldsymbol{B} = \begin{bmatrix} \boldsymbol{b}_1 & \boldsymbol{b}_2 & \dots & \boldsymbol{b}_n \end{bmatrix}, n \ll k$$

$$\boldsymbol{b}_1 = \boldsymbol{A}\boldsymbol{x}_{\sigma(1)}, \dots, \boldsymbol{b}_k = \boldsymbol{A}\boldsymbol{x}_{\sigma(k)},$$

where σ denotes the permutation that orders the vectors in accordance with the chosen norm. The above is called a greedy approximation, and furnishes an alternative to the SVD that exhibits an ordering property. As in the Krylov case, it is usually more efficient to use an orthogonal set obtained through QR factorization

$$\boldsymbol{Q}_n \boldsymbol{R} = \boldsymbol{B}_n.$$

CHAPTER 6

EIGENPROBLEMS

DATA STABILITY

$$A = U\Sigma V^T \quad A = QR \quad A = LU$$

1. The eigenvalue problem

- Consider square matrix $A \in \mathbb{R}^{m\times m}$. The eigenvalue problem asks for vectors $x \in \mathbb{C}^m$, $x \neq 0$, scalars $\lambda \in \mathbb{C}$ such that

$$Ax = \lambda x \tag{6.1}$$

- Eigenvectors are those special vectors whose direction is not modified by the matrix A

- Rewrite (1): $(A - \lambda I)x = 0$, and deduce that $A - \lambda I$ must be singular in order to have non-trivial solutions $\det(A - \lambda I) = 0$

- Consider the determinant

$$\det(A - \lambda I) = \begin{vmatrix} a_{11} - \lambda & a_{12} & \dots & a_{1m} \\ a_{21} & a_{22} - \lambda & \dots & a_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mm} - \lambda \end{vmatrix}$$

- From determinant definition ``sum of all products choosing an element from row/column''

$$\det(A - \lambda I) = (-1)^m \lambda^m + c_1 \lambda^{m-1} + \dots + c_{m-1}\lambda + c_m = p_A(\lambda)$$

is the characteristic polynomial associated with the matrix A, and is of degree m

- $A \in \mathbb{R}^{m\times m}$ has characteristic polynomial $p_A(\lambda)$ of degree m, which has m roots (Fundamental theorem of algebra)

- Example

```
octave] theta=pi/3.; A=[cos(theta) -sin(theta); sin(theta) cos(theta)]
A =

   0.50000  -0.86603
   0.86603   0.50000
```

```
octave] eig(A)
ans =

   0.50000 + 0.86603i
   0.50000 - 0.86603i

octave] [R,lambda]=eig(A);
octave] disp(R);
   0.70711 + 0.00000i   0.70711 - 0.00000i
   0.00000 - 0.70711i   0.00000 + 0.70711i
octave] disp(lambda)
Diagonal Matrix

   0.50000 + 0.86603i                   0
                   0   0.50000 - 0.86603i
octave] A=[-2 1 0 0 0 0; 1 -2 1 0 0 0; 0 1 -2 1 0 0; 0 0 1 -2 1 0; 0 0 0 1 -2 1; 0 0 0 0
        1 -2];
octave] disp(A)
  -2   1   0   0   0   0
   1  -2   1   0   0   0
   0   1  -2   1   0   0
   0   0   1  -2   1   0
   0   0   0   1  -2   1
   0   0   0   0   1  -2
octave] lambda=eig(A);
octave] disp(lambda);
  -3.80194
  -3.24698
  -2.44504
  -1.55496
  -0.75302
  -0.19806
octave]
```

- For $A \in \mathbb{R}^{m \times m}$, the eigenvalue problem 5 ($x \neq 0$) can be written in matrix form as

$$AX = X\Lambda, X = (x_1 \dots x_m) \text{ eigenvector}, \Lambda = \text{diag}(\lambda_1, \dots, \lambda_m) \text{ eigenvalue matrices}$$

- If the column vectors of X are linearly independent, then X is invertible and A can be reduced to diagonal form

$$A = X\Lambda X^{-1}, A = U\Sigma V^T$$

- Diagonal forms are useful in solving linear ODE systems

$$y' = Ay \Longleftrightarrow (X^{-1}y) = \Lambda (X^{-1}y)$$

- Also useful in repeatedly applying A

$$u_k = A^k u_0 = AA \ldots A u_0 = (X\Lambda X^{-1})(X\Lambda X^{-1}) \ldots (X\Lambda X^{-1}) u_0 = X\Lambda^k X^{-1} u_0$$

- When can a matrix be reduced to diagonal form? When eigenvectors are linearly independent such that the inverse of X exists

- Matrices with distinct eigenvalues are diagonalizable. Consider $A \in \mathbb{R}^{m \times m}$ with eigenvalues $\lambda_j \neq \lambda_k$ for $j \neq k$, $j, k \in \{1, \ldots, m\}$

  Proof. By contradiction. Take any two eigenvalues $\lambda_j \neq \lambda_k$ and assume that x_j would depend linearly on x_k, $x_k = cx_j$ for some $c \neq 0$. Then

$$\begin{aligned} Ax_1 = \lambda_1 x_1 &\implies Ax_1 = \lambda_1 x_1 \\ Ax_2 = \lambda_2 x_2 &\implies Acx_1 = \lambda_2 cx_1 \end{aligned}$$

  and subtracting would give $0 = (\lambda_1 - \lambda_2)x_1$. Since x_1 is an eigenvector, hence $x_1 \neq 0$ we obtain a contradiction $\lambda_1 = \lambda_2$.

- The characteristic polynomial might have repeated roots. Establishing diagonalizability in that case requires additional concepts

DEFINITION 6.1. *The algebraic multiplicity of an eigenvalue λ is the number of times it appears as a repeated root of the characteristic polynomial $p(\lambda) = \det(A - \lambda I)$*

Example. $p(\lambda) = \lambda(\lambda - 1)(\lambda - 2)^2$ has two single roots $\lambda_1 = 0$, $\lambda_2 = 1$ and a repeated root $\lambda_{3,4} = 2$. The eigenvalue $\lambda = 2$ has an algebraic multiplicity of 2

DEFINITION 6.2. *The geometric multiplicity of an eigenvalue λ is the dimension of the null space of $A - \lambda I$*

DEFINITION 6.3. *An eigenvalue for which the geometric multiplicity is less than the algebraic multiplicity is said to be defective*

PROPOSITION 6.4. *A matrix is diagonalizable is the geometric multiplicity of each eigenvalue is equal to the algebraic multiplicity of that eigenvalue.*

- Finding eigenvalues as roots of the characteristic polynomial $p(\lambda) = \det(A - \lambda I)$ is suitable for small matrices $A \in \mathbb{R}^{m \times m}$.
  - analytical root-finding formulas are available only for $m \leqslant 4$
  - small errors in characteristic polynomial coefficients can lead to large errors in roots

- Octave/Matlab procedures to find characteristic polynomial
  - `poly(A)` function returns the coefficients
  - `roots(p)` function computes roots of the polynomial

```
octave] A=[5 -4 2; 5 -4 1; -2 2 -3]; disp(A);
   5  -4   2
   5  -4   1
  -2   2  -3
octave] p=poly(A); disp(p);
   1.00000   2.00000  -1.00000  -2.00000
octave] r=roots(p); disp(r');
   1.0000  -2.0000  -1.0000
octave]
```

- Find eigenvectors as non-trivial solutions of system $(\boldsymbol{A}-\lambda\boldsymbol{I})\boldsymbol{x}=0$

$$\lambda_1=1\Longrightarrow \boldsymbol{A}-\lambda_1\boldsymbol{I}=\begin{pmatrix}4&-4&2\\5&-5&1\\-2&2&-4\end{pmatrix}\sim\begin{pmatrix}-2&2&-4\\0&0&-6\\5&-5&1\end{pmatrix}\sim\begin{pmatrix}-2&2&-4\\0&0&-6\\0&0&0\end{pmatrix}$$

  Note convenient choice of row operations to reduce amount of arithmetic, and use of knowledge that $\boldsymbol{A}-\lambda_1\boldsymbol{I}$ is singular to deduce that last row must be null

- In traditional form the above row-echelon reduced system corresponds to

$$\begin{cases}-2x_1+2x_2-4x_3&=&0\\0x_1+0x_2-6x_3&=&0\\0x_1+0x_2+0x_3&=&0\end{cases}\Longrightarrow \boldsymbol{x}=\alpha\begin{pmatrix}1\\1\\0\end{pmatrix},\ \|\boldsymbol{x}\|=1\Longrightarrow\alpha=1/\sqrt{2}$$

- In Octave/Matlab the computations are carried out by the null function

```
octave] null(A+5*eye(3))'
 ans = [](0x3)
octave]
```

- The eigenvalues of $\boldsymbol{I}\in\mathbb{R}^{3\times3}$ are $\lambda_{1,2,3}=1$, but small errors in numerical computation can give roots of the characteristic polynomial with imaginary parts

```
octave> lambda=roots(poly(eye(3))); disp(lambda')
   1.00001 - 0.00001i   1.00001 + 0.00001i   0.99999 - 0.00000i
octave>
```

- In the following example notice that if we slightly perturb $\boldsymbol{A}$ (by a quantity less than 0.0005=0.05%), the eigenvalues get perturb by a larger amount, e.g. 0.13%.

```
octave] A=[-2 1 -1; 5 -3 6; 5 -1 4]; disp([eig(A) eig(A+0.001*(rand(3,3)-0.5))])
   3.0000 + 0.0000i   3.0005 + 0.0000i
  -2.0000 + 0.0000i  -2.0000 + 0.0161i
  -2.0000 + 0.0000i  -2.0000 - 0.0161i
octave]
```

- Extracting eigenvalues and eigenvectors is a commonly encountered operation, and specialized functions exist to carry this out, including the `eig` function

```
octave>  [X,L]=eig(A); disp([L X]);
  -2.00000   0.00000   0.00000  -0.57735  -0.00000   0.57735
   0.00000   3.00000   0.00000   0.57735   0.70711  -0.57735
   0.00000   0.00000  -2.00000   0.57735   0.70711  -0.57735
octave> disp(null(A-3*eye(3)))
   0.00000
   0.70711
   0.70711
octave> disp(null(A+2*eye(3)))
   0.57735
  -0.57735
  -0.57735
octave>
```

- Recall definitions of eigenvalue algebraic m_λ and geometric multiplicities n_λ.

DEFINITION. *A matrix which has $n_\lambda < m_\lambda$ for any of its eigenvalues is said to be defective.*

```
octave> A=[-2 1 -1; 5 -3 6; 5 -1 4]; [X,L]=eig(A); disp(L);
Diagonal Matrix

  -2.0000        0        0
       0   3.0000        0
       0        0  -2.0000
octave> disp(X);
  -5.7735e-01  -1.9153e-17   5.7735e-01
   5.7735e-01   7.0711e-01  -5.7735e-01
   5.7735e-01   7.0711e-01  -5.7735e-01
octave> disp(null(A+2*eye(3)));
   0.57735
  -0.57735
  -0.57735
octave> disp(rank(X))
 2
octave>
```

2. Computation of the SVD

- The SVD is determined by eigendecomposition of A^TA, and AA^T
  - $A^TA = (U\Sigma V^T)^T(U\Sigma V^T) = V(\Sigma^T\Sigma)V^T$, an eigendecomposition of A^TA. The columns of V are eigenvectors of A^TA and called right singular vectors of A

$$B = A^TA = V\Sigma^T\Sigma V^T = V\Lambda V^T$$

  - $AA^T = (U\Sigma V^T)(U\Sigma^T V^T)^T = U(\Sigma\Sigma^T)U^T$, an eigendecomposition of A^TA. The columns of U are eigenvectors of AA^T and called left singular vectors of A
  - The matrix Σ has form

$$\Sigma = \begin{pmatrix} \sigma_1 & & & & & \\ & \sigma_2 & & & & \\ & & \ddots & & & \\ & & & \sigma_r & & \\ & & & & 0 & \\ & & & & & \ddots \end{pmatrix} \in \mathbb{R}_+^{m\times n}$$

    and σ_i are the singular values of A.

- The singular value decomposition (SVD) furnishes complete information about A
  - $\operatorname{rank}(A) = r$ (the number of non-zero singular values)
  - U, V are orthogonal basis for the domain and codomain of A

DATA RESONANCE

1. Bases induced by eigenmodes

The trigonometric functions $\{1, \cos t, \sin t, \cos 2t, \sin 2t, \ldots\}$ have been introduced as a particularly appropriate basis for periodic functions. The functions $\cos(kt), \sin(kt)$ are also known as solution of the homogeneous differential equation

$$y'' + k^2 y = 0.$$

The diferential operator is a linear mapping

$$\frac{\mathrm{d}^q}{\mathrm{d}t^q}(\alpha y + \beta z) = \alpha\frac{\mathrm{d}^q y}{\mathrm{d}t^q} + \beta\frac{\mathrm{d}^q z}{\mathrm{d}t^q},$$

and hence has an associated linear mapping. An approximation of the second-order differentiation operation is given by the finite difference formulas

$$y_i'' = y''(t_i) \cong \frac{1}{h^2}(y_{i+1} - 2\,y_i + y_{i-1})$$

```
octave]
```